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Facts & Figures

Chemistry & Materials Science Directorate Honoring the Laboratory's 50th Year, 2002

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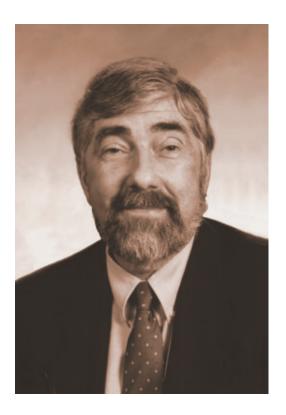
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Message from Hal Graboske

Facts & Figures has evolved over the years to keep pace with the growth of the CMS Directorate. The title of this publication reflects its origins and intent—to be a broad overview of budgetary, personnel and other administrative information about Lawrence Livermore National Laboratory (LLNL). This year, to complement this information, we expanded the contents to include a wider-range of subject matter. Facts & Figures 2002 summarizes our scientific and technical accomplishments to acknowledge the scientific achievements and the multidisciplinary teams that make the science happen—which is the cornerstone of the Directorate's success.

In addition, as a special tribute to the Laboratory's 50 years of excellence, *Facts & Figures* 2002 also honors the Institution, its Directors, and Chemistry and Materials Science and its Associate Directors. Each of us is responsible for making this Institution flourish—reflecting on the past gives us an opportunity to take pride in our accomplishments, to review our goals, and to plan for a dynamic future.

A special thank you to Denise Robinson for her inspiration to enhance the *Facts & Figures* publication—a tribute to the Directorate's vitality and continued desire to explore new ideas and make them happen.

1

The wisdom of a dynamic past prepares us for a challenging future

It was the end of World War II, the beginning of a new war with North Korea, and a new era of uncertainty—the Soviet Union had just exploded their first atomic bomb in August of 1949. Ernest O.



Lawrence, the Director of what was then called the University of California Radiation Laboratory (UCRL), had grave concerns about the possibility that the Soviets would rapidly proceed with the development of the hydrogen bomb. Sharing this concern was Edward Teller, who had worked at the Los Alamos Laboratory during the war, and who had, in 1949, headed the project there which was exploring the possibility of producing a

thermonuclear device. Lawrence and Teller, sharing a passion for science and a dedication to the United States, wanted to respond to these uncertain times in a direct and useful way. They met in October of 1949 to discuss their concerns about the Soviet atomic detonation. Teller also believed that friendly competition for Los Alamos—the only weapons laboratory in the United States at the time—would accelerate the development of thermonuclear weapons and fuel scientific accomplishments. In the summer of 1952, at an abandoned Naval Air Station in Livermore, a branch of the UCRL was created—an outgrowth of America's ominous times.

Building an Institution...

Ernest O. Lawrence, co-founder of this new Laboratory, designated Herbert F. York, then 32 years old, to develop the plans for what was initially called Project Whitney, and to run the project when it began. The plan York developed called for four activities: the design of thermonuclear devices, diagnostic measurements on weapons experiments for Los Alamos and for devices developed at Livermore, work on controlled thermonuclear reactions for potential power sources, and basic physics research. To implement the plan required people and facilities. In the Chicago Conrad Hilton Hotel, York outlined the research and bare-bones UCRL organizational structure for the diagnostic work and design efforts—the first pieces of the Laboratory's blueprint. Many of the people initially came from the staff of the Radiation Laboratory in Berkeley, others were graduate students with degrees in Physics, Chemistry, and Engineering. When work started in Livermore in September of 1952, there were approximately seventy people on staff. York's conceptual ideas led to rapid growth reaching a total of 658 employees by July 1953—an increase way beyond their expectations. Ernest Lawrence was the Director of the Laboratory, and Herb York, who had no title, reported to him...

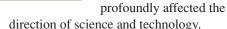
As York recalled Ernest saying, "Herb, you go out there and run the place." According to York, "an amusing thing happened repeatedly during the first year and a half. I did all the negotiating with Washington about the program; nobody else, neither Edward nor any of the others. It just was a simpler world. And whenever I would be there, people... ...would say. 'Who is Mr. Livermore?' Or, 'Who is the Director of the Laboratory there?' And I'd say, 'Ernest told me to go



out there and run the thing.' And I would sign these letters, which were very important letters, the plan for the next year, year and a half, with no title, just my name. I'd sign them Herbert York, UCRL, Livermore, but no title. And they were the letters that established the program of the Laboratory..."

In 1958 Ernest Lawrence died, and the Regents of the University of California renamed the Radiation Laboratory the Lawrence Radiation Laboratory. Herb York left the Laboratory to become the Director of Defense Research and Engineering in the Department of Defense, and Edward Teller

became the new Director of the Livermore site. Teller's own inclination was to pursue pure science, but his appointment as Director came after an untimely helicopter accident took the life of Mark Mills, who some believe was being groomed to take Herb York's place as Director. Prolific in his ideas and determined in his pursuit of scientific truth, Teller, then and now, has promoted groundbreaking scientific studies that often have



In 1958, a three-year moratorium on nuclear testing began, and peaceful applications for nuclear explosives became the new direction at the Laboratory. Harold Brown, who succeeded Teller as Director,



Edward Teller

Co-Founder, Director, 1958-60

Harold BrownDirector, 1960–61

faced a different challenge—layoffs were a possibility, creating volatility and uncertainty. Brown was instrumental in securing the Pluto project, a spinoff of the Rover project at Los Alamos, that successfully kept talented people at the Laboratory. It was a different field of work from nuclear weapons, but still in the nuclear field. The objective was to develop a reactor which would be the

power source for an unmanned, supersonic, very low altitude (mach 3 at 500 ft) ramjet aircraft with exceedingly long range—tens of thousands of miles. The program was ultimately cancelled due to a lack of mission requirements by the military for such a system.

During the ten years that followed, two different directors led the Laboratory. It was a decade when efforts were strongly concentrated on the requirements of the strategic missile systems. The Laboratory's focus was on developing warheads for the second generation Polaris system and the more advanced Poseidon and design teams were developing the Minutemen warheads.

John Foster, Director for nearly half of this decade (1961–65), rode the winds of the

60s—from a moratorium on nuclear testing to the Soviet's resumption of testing; from President Kennedy's challenge over the Cuban crisis to a treaty that banned aboveground atmospheric tests and birthed underground testing. This was an exciting time for the Laboratory because underground testing was a more fertile environment for capturing data. The Laboratory also entered a new field with the establishment of the



John S. Foster
Director, 1961–65

Biomedical program to investigate the effects of radioactive isotopes on living systems.

Michael May, who became Director the last half of this decade (1965–71), led the Laboratory through the mid-60s—a time when protests began to peak across the nation. May faced difficult issues and threats of layoffs—funding had shrunk, the Laboratory was in the eye of anti-nuclear demonstrations, and America was challenging itself. May's skillful management style held things together during simultaneous talks of whether the University of California should manage the Laboratory—the outcome of which separated the administration of Lawrence Berkeley and LLNL.



Michael M. May Director, 1965–71

According to Michael May, sometime in 1952...

"...I heard of the place [the Laboratory] from Herb York.....I asked Herb what the place was about and he said, 'I can't tell you, but I'll tell you a couple of things about it. First, it's interesting enough to attract people like von Neumann, Teller, Wheeler (and he mentioned some others). Second, it's permanent work, and by permanent I mean five yearish.' I had no idea what the Lab would be

about....Livermore was just a sign on Highway 50 to me on the way to Los Angeles or Pasadena..."

The turmoil of the 60s came to a close, and the Laboratory had new leadership under Roger Batzel from 1971 to 1988. Although the Laboratory experienced a small decline of workers in the early 70s, the last half of the



Director, 1971–88

decade saw the number of employees rise steadily beyond 6,000. Dozens of new office buildings, laboratories, and research facilities were erected; biomedical, energy, and environmental programs were expanded; and laser science grew dramatically with the dedication of the Shiva and Nova lasers. The 70s focus of the weapons work shifted to tactical systems, such as short-range, surface-tosurface missiles, and

artillery shells. Despite the Laboratory's substantial diversification, Roger kept the main focus on strengthening the nation's forces for nuclear deterrence. He had a particular genius for choosing the right leaders for the Laboratory's major research efforts and supporting them in attaining the resources they needed to succeed.

Following this era of expansion, the Laboratory continued the development of warheads for new military systems as John Nuckolls took the helm as Director from 1988

to 1994. At the same time, studies at the Laboratory created the first laboratoryscale x-ray lasers and developed nuclear powered x-ray lasers for possible applications to strategic defense. During those same years many changes were taking place—the dissolution of the Soviet Union, the end of the Cold War and tearing down the Berlin Wall, and a domestic legislative amendment that ended nuclear testing in 1992—all which changed



Director, 1988–94

the role of the Laboratory, dramatically. The horizons looked peaceful.

In 1994, John Nuckolls passed the leadership torch to Bruce Tarter. A new century was looming, and the Laboratory was wrestling with questions related to the nuclear stockpile. The National Ignition Facility, which would be the world's largest laser, was being proposed to address some of the stockpile issues. No facility in the history of the Laboratory had triggered the level of publicity, public and Congressional scrutiny, and sheer scientific excitement. Upon completion, the NIF will play a significant role

in the science-based Stockpile Stewardship Program to assure the safety and reliability of the nation's nuclear weapons. The facility will also be used to research inertial confinement fusion energy and basic science such as astrophysics and materials under extreme conditions of temperature pressure and strain rates.



C. Bruce Tarter Director, 1994–present

In the late 90s, the Laboratory found itself in a rapidly changing environment—times were tough and attention was being diverted from the day-to-day technical work associated with core missions to issues involving security—the handling and protection of classified information; safety—the development and implementation of a complex-wide integrated safety management plan; and diversity ensuring and valuing a diverse workforce. At the same time, the U.S. economy was booming and pressure from the outside began to lure away key elements of the Laboratory's technical staff. Complicating this new landscape was the establishment of the National Nuclear Security Administration (NNSA), an autonomous organization within the Department of Energy, and new provisions within the University of California's contract—all creating a mood of uncertainty.

And now, at the birth of a new century and a new millennium, the tragedy of September 11, 2001—an unprecedented event in American history, a threat to freedom-loving people worldwide, and a domestic loss of life unparalleled. So what is the Laboratory's role in these toughest of times? One cannot help but reflect on how the passion, inspiration, and courage of those that began this great institution somehow planted a seed that can only produce the finest solutions. Since September 11, a pouring out of scientific achievement and outstanding advancements in state-of-the-art technologies have been there to meet the needs of our great nation. And, a willingness prevails to get through this and to move forward.

Have we come full circle...

The events that made up the early stages of World War II brought about the creation of the Laboratory and stimulated an era of dynamic growth and change. With the nation at peace, the byproducts of the nuclear era led to multiple programs and successes. Now, a half-century later, we have come full circle in many ways. We face another dark hour that thrusts the Laboratory into a different ominous war—terrorism and its many faces. The challenge is great, but history is on our side—the passion, the dedication, and the talent of this institution and its staff will move us forward into a prosperous and peaceful future, once again.

—Dabbie Schleich

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We've Come a Long Way...

In 1952, Chemistry began its laboratory operations in the barracks building of the Naval Air Station. Herb York, the Director of the Laboratory, had his offices in the dispensary and processing experiments were conducted in the ladies' room. A few years later, radiochemistry diagnostics were performed in Building 101 (later renamed Building 222) the first permanent building of the University of California Radiation Laboratory (UCRL). Since then, the buildings and the programs have expanded with state-of-the-art sophistication and the name of the Directorate has changed many times, but the common theme and determination to "do great science" has remained constant. The mission of Chemistry and Materials Science (CMS) continues—to support national security and to push the frontiers of science.

Ken Street joined the Laboratory in 1952, hired to create a chemistry department to support the fledgling weapons program. One year later, a fellow young scientist from the

California Research and Development Corporation, Roger Batzel, joined as Street's assistant. In 1956, the UCRL-Livermore scientific divisions were formally established, and in 1957, Street became the Associate Director of Chemistry. The Chemistry Department was narrowly focused at the time on strictly weapons work involving chemistry that needed to be done to field and diagnose devices. The special materials used in nuclear weapons—high explosives, plutonium, uranium, beryllium and tritium to name a few-were all within the purview and expertise of the Laboratory's first chemists. The Department was involved in the search for new high explosives materials and the development of materials for particular applications, such as the Pluto Program, and maintaining its major emphasis to contribute to the Test Program in terms of radiochemical diagnostics.

In 1961, Roger Batzel succeeded Street as Associate Director for Chemistry. This was the start of significant changes in his responsibilities, leading to his legacy of excellence at the Laboratory. The Pluto project

The mid- to late-50s . . .



Some of the Chemistry participants in the 1956 Redwing Operations at the Bikini and Enewetak Atolls.



Harry Hicks ready to board an Air Force RB-57 sampling plane during the 1958 Hardtack Operations at the Bikini and Enewetak Atolls.

came and went with B-52s and missiles to displace this ramjet concept. Operation Plumbbob became Chemistry's first test experience through radiochemistry to measure the yields. The Laboratory also went to a six-day work week. According to Batzel...

In some of the situations it turned out to be seven-day workweeks. You had these atmospheric tests and you were tied pretty close to a schedule because it interacted with a lot of other things going on at the same time and if the Chemistry Department had the responsibility of providing a finished part that had to be part of the explosive then the Chemistry Department would work as long as required.

As the Laboratory was growing, so were the elements of Chemistry to support these dynamic changes. Chemistry's programmatic work and research evolved from Project Whitney to its continuous search today for new elements in the Periodic Table. This includes projects like the Hutch event in 1969 and a long collaboration with the Joint Institute for Nuclear Research in Dubna, Russia that has

resulted in the recent discovery of elements 114 and 116. Materials science advanced from defining types and classes of materials—metallurgy, ceramics, and polymers, to a broader focus on synthesis, processing and characterization, shifting toward complex materials and systems. The theme for nearly all Chemistry's new materials became lighter, stronger, and tougher. Current materials are being developed with unique properties that are specifically designed for a particular application—combining theory with experiment to understand the materials at a more fundamental level than ever before.

In 1965, the Chemistry Department acquired its first digital computer dedicated to chemistry applications. Operating in a timeshare mode, the computer was able to control a variety of experimental equipment, simultaneously. Over the next two decades, Chemistry helped the Laboratory pioneer ways of using more and more advanced computers to control chemical instrumentation.

The late-50s to mid-60s . . .



Ken StreetAssociate Director, 1957–61



Members of the Chemistry group relax during a lull in testing. Hardtack Operations, 1958, Bikini and Enewetak Atolls.



From the mid-60s to the late 70s. Chemistry had several leaders. Gus Dorough became the Department Head of Chemistry in 1967, succeeded by James Kane in 1971 when Dorough accepted a position with the Department of Defense as Director of Defense Research and Engineering in Washington D.C. In 1973, Dorough returned to the Laboratory and took over as Associate Director for Scientific Support, overseeing the Chemistry Department and the Computations Department. When Kane resigned in 1974 to accept a position as Technical Assistant to the USAEC General Manager in Washington, D.C., Jack Frazer took his place as Head of Chemistry. In 1977, the Radiochemistry Division became part of the Test Program Directorate under Associate Director Rich Wagner to create a more visible organization. The Radiochemistry Division, also known as the Nuclear Chemistry Division, remained in that directorate until the end of nuclear testing, when it was recombined with Chemistry in 1994. Charles Bender followed Jack Frazer as Head of Chemistry in 1978, leaving a legendary tale behind. Bender,

known for his love of computers, used to carry a cardboard box full of IBM punch cards where ever he went—just in case an opportunity arose to sneak away and "do real work".

In the early 70s, Laboratory personnel, under the leadership of the Radiochemistry Division and the Biomedical Division, returned to the Pacific Atolls of Enewetak and Bikini to conduct radiological surveys of soils, plants and the marine environment before inhabitants could return to the island. Later, in 1978, when the Russian nuclear-powered satellite, Cosmos 954, re-entered the earth's atmosphere and burned over Canada's Northwest territories, Chemistry's metallurgists and radiochemists were called upon again as key participants in Operation Morninglight.

As a result of a congressional amendment to the AEC charter in 1971, which allowed the three weapons laboratories to become engaged in non-nuclear research, Chemistry initiated new programs to address the energy crisis. These programs included work on battery research, oil shale, coal gasification and geothermal energy.

The mid-60s to late-70s...



Gus Dorough

Department Head, 1967–71

Associate Director, 1973–82



James S. Kane Department Head, 1971–74



Jack W. Frazer
Department Head, 1974–78

In the mid-70s, the triple-quadrupole mass spectrometer (TQMS) was designed—
Chemistry's most advanced computercontrolled instrument. It was capable of operating in five different modes, performing mass-spectroscopic analysis of ions previously selected by a conventional quadrupole mass spectrometer. Also emerging was the Laser Fusion Program.

In 1985, Chris Gatrousis was named Associate Director for CMS. In 1987, the Weapons Materials Research & Development Facility (Building 235) was dedicated, becoming the first materials science facility. The High-Explosives Application's Facility (Building 191) was also established jointly with the Laboratory's Weapons Program to study chemical high explosives. The mid- to late-80s became the era of CMS discovering metal-oxide super conductors, multilayers, aerogels, nuclear fission, and insensitive high explosives. Multilayers have the potential for extremely high mechanical performance, offering extraordinary strength, hardness, heatresistance, and unexpected new properties and are among the first materials to be

designed and fabricated at the atomic level. Aerogels, a fascinating sponge-like foam also called "frozen smoke", can support 1600 times its own weight. Their complicated, cross-linked internal structure gives them the highest internal surface area per gram of material of any known material. Their use has expanded from national security applications, to NASA satellites, and widespread interest from industry. The discovery of bimodal fission significantly changed the way theoreticians modeled the fission process and led to new knowledge of how heavy nuclear matter behaves.

In 1989, CMS surveyed the field of research in the heaviest elements and concluded that the supply of trained professionals was diminishing to the detriment of national goals. A mechanism was needed to promote, expand, and strengthen basic and applied understanding of the properties of elements heavier than actinium. To achieve this goal, the concept of forming an institute dedicated to research and training of scientists in the chemistry and physics of the heaviest

The late-70s to mid-80s . . .





Deputy Director Jack Kahn (left) with Klaus Ernst, Analytical Chemistry Division Leader, and Charles Bender, CMS Department Head. Photo taken in the early 1980s.

elements was explored at a workshop held in 1990 at the Claremont Hotel in Oakland, which included national and international leaders in the field. After further discussions with LLNL management and colleagues and Professors G. T. Seaborg and D. C. Hoffman at Lawrence Berkeley Laboratory, LLNL's Glenn T. Seaborg Institute for Transactinium Science was formed. The institute emphasizes education and training as well as research and development in the science and technology of the heavy elements. CMS also developed a particularly strong postdoctoral program where high standards are set for its participants and new ideas are spawned. Later, during Hal Graboske's leadership, the program was expanded to include additional nuclear science competencies.

Safer, less sensitive high explosives were developed that have significantly improved the safety and survivability of munitions, weapons, and personnel. TATB (1,3,5-triamino-2,4,6-trinitrobenzene) is nearly invulnerable to significant energy release in plane crashes, fires, and explosions or to deliberate attack with small arms fire. The

involvement with energetic materials of course began in 1952, but these capabilities have, over the years, expanded dramatically to advanced conventional weapons, rockets and propellants, antiterrorist work, demilitarization, and industrial applications.

The last decade of the 20th century sharpened CMS' mission and its purpose, playing a vital role in the success of Laboratory programs. Jeff Wadsworth succeeded Chris Gatrousis in 1994, followed by Larry Newkirk as acting Associate Director until 1997 when Harold Graboske took the leadership role. With Hal Graboske's direction came a new vision for the Directorate. His approach to leading CMS was to re-examine the Directorate's goals and to align CMS along with the Laboratory's strategic direction. This vision prepared CMS for a new century and a new kind of reality.

During the 90s, the National Ignition Facility (NIF) moved from the drawing board to construction—essential for the Department of Energy's Stockpile Stewardship and Management Program. With the advent of the powerful atomic-force microscope, Livermore

The mid-80s to early-90s . . .



Christopher GatrousisAssociate Director, 1985–93



Physicist Bob Meisenheimer (right) describes some of the metallurgical capabilities to CMS AD Chris Gatrousis (left), Jo Ann Elferink, Manager of DOE Oakland Operations, Troy Wade, DOE Assistant Secretary for Defense Programs, Associate Directors Bob Godwin, Phil Coyle, George Miller, and Lab Director Roger Batzel, following ceremonies at the dedication of Bldg. 235, in 1987.

researchers began to elucidate the growth mechanisms and three-dimensional structures of widely different solution-based crystals on the nanometer (billionth-of-a-meter) scale. Much of the crystal development work has centered on the need to better understand KDP crystal growth because of its direct impact on the NIF. CMS also co-developed a revolutionary process of producing meterscale plates of laser glass at a rate 20 times faster and 5 times cheaper to meet the demands of the NIF laser. The Continuous Laser Glass Melting Process converts highpurity, powdered raw materials into one continuously moving strip of high-opticalquality laser glass. Many of the technical barriers that NIF must overcome are materials related. Therefore, CMS has a significant role to play in helping the NIF achieve this goal.

CMS scientific and technical staff have contributed significantly to the success of programs in the Nonproliferation, Arms Control, and International Security Directorate (NAI), since it was formed in 1992. The staff members of the Laboratory's

Forensic Science Center, which had its early beginnings in CMS' Analytical Sciences Division in 1991 before moving to NAI, have become leaders in the development of special technologies for law enforcement, national security, defense, and intelligence applications. CMS provides expertise in organic, inorganic, nuclear chemistry, and biological chemistry to analyze the composition and address questions about the source of a wide range of samples of material. Since the September 11, 2001 terrorist incident, this expertise has been in particularly high demand. In addition, chemical engineers from CMS are contributing their skills in process analysis to the development of NAI's Counterproliferation Analysis and Planning System (CAPS), a versatile and powerful tool for analyzing the proliferation activities of foreign countries. These analyses provide valuable technical input to the decisionmaking agencies and individuals with responsibility for determining the U.S. response to proliferation activities. Also, CMS nuclear scientists are contributing their

The mid-90s . . .



Jeffrey Wadsworth Associate Director, 1994–96



AD Jeff Wadsworth and Denise Robinson, Chair of the Laboratory's 1994 Home Campaign, present awards to Phil Schultz and Steve Hunt.

skills in radiation detection, gamma-ray spectrometry, and mass spectrometry to NAI's programs in the prevention of nuclear proliferation by providing technologies and expertise to cooperative international programs associated with treaties and other agreements. For example, sophisticated codes originally developed in the Nuclear Chemistry Division to analyze the complex gamma-ray emissions from nuclear explosion debris now form the international standard for the analysis of samples collected by the International Atomic Energy Agency (IAEA) and other international organizations. In related work, CMS expertise is contributing significantly to NAI activities to help various Russian sites improve the protection of their fissile materials through the NNSA Material Protection, Control, and Accounting (MPC&A) Program. The development of new radiation detection technologies is also important to NAI programs, and CMS nuclear scientists are developing cutting-edge gamma-ray imaging technologies that can be applied to a range of counterterrorism applications.

Major facility changes began during the 90s—the quality of the infrastructure needed to match the advances in scientific achievement. It was time to replace the old with the new and revitalize, where appropriate. After 50 years of service, CMS migrated from Building 222 to Building 132 North, which became the icon for chemistry laboratories certainly a transition from Chemistry's beginnings—from processing experiments in the ladies' room to highly sophisticated stateof-the-art laboratories. CMS created the Space Action Team (SAT) to safely complete the migration and consolidation. SAT is still very active in this area, with decommissioning, deactivation, decontamination and demolition (D&D) projects in process for the Atomic Vapor Laser Isotope Separation (AVLIS) facilities and the demolition of Building 222. Buildings 151 and 241 were re-roofed, and the Isotope Sciences Facility Line Item is underway and progressing well to revitalize Buildings 151 and 154, to clear legacy material in Building 241, and to add a new office space (Building 155) adjacent to the

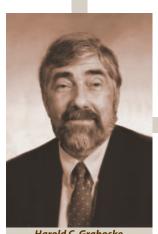
The mid- to late-90s . . .



Acting Assoc. Director, 1996–97



Acting AD Larry Newkirk presents the 1996 Home Campaign's contribution award to Trish Baisden, Analytical Sciences Division Leader, and Sid Niemeyer, Isotope Sciences Division Leader.



Harold C. GraboskeAssociate Director, 1997–present

Isotope Sciences Facility (B151). Looking forward, CMS is working with the weapons program to design a new processing area at Site 300 and plan for a modern materials facility at Site 200—all changes to keep pace with the advancing frontiers.

And there are great hopes for the future...

Guiding the development of new disciplinary capabilities and innovations is especially challenging at a time when national expectations of our Laboratory are changing rapidly. The goal is to provide the right people and a research environment that fosters growth. CMS is well positioned to meet the changing needs and emerging opportunities of the years to come. From continued support of the Laboratory's weapons program to dealing with the nation's recent threat of terrorism—the CMS Directorate remains at the cutting-edge of scientific discovery.

—Dabbie Schleich

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S&TR, August 1995. Commentary by Jeffrey Wadsworth.

—, June 1997, September 1999, December 2000. *Commentary by Hal Graboske*.

K. Street, Archival Interview, 1982.

to the present ...



AD Hal Graboske observes Don Daronco's performance as Chef at the CMS 2000 picnic.



Hal Graboske and Doug Marden at the 2000 pancake breakfast and awards ceremony in honor of the successful implementation of Integrated Safety Management passing verification.

In Support of the Laboratory's Mission, Vision and Goals

The CMS Directorate supports LLNL's mission—to be a premier applied-science national security laboratory. Its primary mission is to ensure that the nation's nuclear weapons remain safe, secure, and reliable and to prevent the spread and use of nuclear weapons worldwide. The mission enables Laboratory programs in advanced defense technologies, energy, environment, biosciences, and basic science to apply their unique capabilities and to enhance the competencies needed for the national security mission.

CMS supports the Laboratory's goal—to apply the best science and technology to enhance the security and well being of the nation and to make the world a safer place. When CMS has achieved its vision, the Laboratory and its Programs will view CMS as a highly valued, relevant partner and as the preeminent partner of effective materials and chemistry solutions required to assure success of their missions. CMS will be the cornerstone of LLNL's nationally recognized excellence for material and chemical sciences to enable the Laboratory's Programs in achieving their mission in national security. CMS will have administrative staff with state-of-the art research and facilities for long-term institutional excellence.

Science and Technology Highlights, Awards and Achievements

The Directorate is proud of its world-class teams that pool varied talents to solve problems related to the Laboratory's mission and achieve recognition for a job well done. The Science & Technology Review (S&TR) publication highlights many of these achievements, many of which also receive specific recognition and awards from the Institution, the Director, and the Directorate. Over the course of a two-year period, the quality of science is also reviewed by the Scientific Advisory Review Committee (SARC) in the context of their relevance to national needs and agency missions. The Committee also addresses programmatic performance and planning, and the performance in the technical development and operation of major facilities. Biographical sketches of the SARC members are shown at the end of this publication.

Science and Technology Highlights

S&TR March 2001—Plutonium Up Close...Way Close. To support stockpile stewardship, a number of experiments are under way to measure the structural, electrical, and chemical properties of plutonium and its alloys and to determine how these materials change over time. Adam Schwartz, Bill Wolfer, and Mark Wall from the Materials Science & Technology Division (MSTD) are pursuing the evolution of damage to plutonium's structure on scales as small as a billionth of a meter. To accomplish this, they use the 300kiloelectronvolt, field-emission transmission electron microscope (TEM) to look directly at the internal structure of materials (see Figure 1). Using samples of plutonium from old, disassembled nuclear warheads and comparing their resulting micrographs to those from newly cast plutonium, the researchers can better determine the kinds and amounts of defects and changes that occur over time.

S&TR June 2001—Turning Carbon
Directly into Electricity. John Cooper from
MSTD is working to develop a method for
producing electricity that is safe, relatively
simple, efficient, and kind to the environment



Figure 1. Microscopist Mark Wall uses the TEM to image the microstructure of plutonium.

(see Figure 2). This direct carbon conversion method converts carbon particles, obtained from different fossil fuels, directly into electricity without the need for such traditional equipment as steam-reforming reactors, boilers, and turbines. If adopted on a large scale, direct carbon conversion would help to conserve precious fossil resources by allowing more power to be harnessed from the same amount of fuel. It would also improve the environment by substantially decreasing the amount of pollutants emitted into the atmosphere per kilowatt-hour of electrical energy that is generated. It would, most importantly, decrease emissions of carbon dioxide, which are largely responsible for global warming.

S&TR June 2001—This Nitrogen
Molecule Really Packs Heat. Riad Manaa in
the Chemistry and Chemical Engineering
Division (CChED) may have found the unusual
nitrogen molecule. His computer simulations
show that it might be possible to join six 10atom nitrogen molecules into a soccer-ballshaped molecule known as
buckminsterfullerne, fullerene, for short. With
their high energy density, large nitrogen
molecules would be prime candidates for new
high explosives or perhaps for a novel
propellant.



Figure 2. Nerine Cherepy and John Cooper assemble an experimental carbon conversion fuel cell.

S&TR June 2001—PEREGRINE Goes to Work. When patients receive radiation therapy, they are bombarded by billions to trillions of particles. PEREGRINE Monte Carlo radiation transport algorithms determine the dose deposited in the patient by following the path of representative particles as they travel through the body. By sampling millions of the trillions of particles that enter the body and recording the energy deposited by each as it travels through the body, PEREGRINE's Monte Carlo statistical method develops an accurate representation of the dose distribution (see Figure 3). PEREGRINE team members have won many awards for their work, and Christine Hartmann-Siantar, added another in February 2000 as one of four first-ever recipients of the Edward Teller Fellowship Award. Working with the team, she is using the fellowship to study how radiation damages DNA.

S&TR November 2001—Welding Science. Over the last several years, MSTD's John Elmer, Joe Wong, and Todd Palmer in collaboration with colleagues at Pennsylvania State University and Oak Ridge National Laboratory have succeeded in producing maps of the microstructural changes that occur in and around the weld area as a metal melts and resolidifies. More recently, their experiments have revealed second-by-second changes in a metal's microstructure during welding. The ultimate purpose of all research on welding is to move useful information out to the welders of the world, to help them make better welds. Elmer was named a Fellow of the American Welding Society in 2000 and, along with Wong and his colleagues at Penn State, also received the prestigious William Spraragen Memorial Award. Their article on modeling of titanium welding was selected the best paper of 2000 in the Welding Journal Research Supplement.

Other Highlighted Research

In a series of investigations over the past five years, a team of Livermore researchers led by Bryant Hudson in CMS has demonstrated the use of a collection of characterization techniques that have revolutionized our ability to track the movement of water in the subsurface. The project seeks to assess and monitor California groundwater and estimate its vulnerability to contamination. The group is the only group in the world currently using separated noble gas isotopes as groundwater tracers. This work is important to the Laboratory because it further enhances LLNL's position as a valuable resource recognized by, and of service to, the State of California. Other research team members include Lee Davisson. Jean Moran, Gail Eaton and Wavne Culham. In addition, two postdoctoral researchers have been important contributors to the group: Jordan Clark, now on the faculty at University of California, Santa Barbara and Brenda Ekwurzel, now on the faculty of the University of Arizona.

Institutional Achievements

During FY00, the Institution inaugurated its first annual Institutional Award to celebrate notable Laboratory achievements in science and technology. Director Bruce Tarter and Deputy Director Jeff Wadsworth presented certificates, special memorabilia, and cash awards of \$1000 to the team members.

CMS and its nuclear physicists from the Analytical and Nuclear Chemistry Division (ANCD) in collaboration with Russian scientists from the Joint Institute for Nuclear Research in Dubna, Russia, were honored for their discovery of a new ultraheavy element element 114. The team was also recognized by both Chemical Engineering News and Popular Science. Using isotopes provided by Livermore, the Russian-U.S. team bombarded a plutonium-244 target with calcium-48 atoms to create the new element. The excitement generated by the discovery stems largely from the stability of the new element, the nucleus of which is believed to consist of 114 protons and 184 neutrons. Unlike other manufactured heavy elements, element 114 is relatively longlived, surviving for 30 seconds—as opposed to mere microseconds—before decaying. The Livermore team is shown in Figure 4.



Figure 3. Christine Hartmann–Siantar, program leader for the PEREGRINE project, is shown with John Friede, chairman and chief executive officer of NOMOS Corporation during the announcement of FDA approval for PEREGRINE.

Director's Awards

The Director and Deputy Director for Science and Technology initiated these awards to prove an opportunity to celebrate the significant accomplishments of the Laboratory's technical staff. These are compelling research efforts symbolic of world-class work of this Laboratory.

Two research teams from CMS received this year's award—the Calcite team and the Laser Glass team (see Figures 5 and 6).

The Calcite team led by Jim DeYoreo in collaboration with scientists from Virginia Polytechnic Institute and the University of South Alabama, developed key insights into a process called biomineralization. This process is key to problems as diverse as biomimetic synthesis of nanostructures, CO₂ sequestration, profiling of paleo-climates, developing tools for astrobiology, and understanding the origin of life on Earth. Using atomic force microscopy (AFM), surface spectroscopy, and molecular modeling, the team investigated the interaction of amino acids and inorganic impurities with CaCO₂ crystal surfaces. The latest results show that individual left- and right-handed amino acids bind preferentially to steps on the surface of calcite that are related by mirror symmetry. This interaction plays a primary role in determining the evolution of crystal shape.



Figure 4. Bruce Tarter (left) and Jeff Wadsworth (right) shown here with Element 114 team members: Kenton Moody, Nancy Stoyer, John Wild, and Ronald Lougheed Team member not shown: Mark Stoyer.



Figure 5. Calcite team (left to right): James De Yoreo, Mary McBride, Christine Orme, Alexsandr Noy (Lawrence Fellow), Theresa Land of CMS. Team members not shown are: Prof. Patricia Dove of Virginia Polytechnic Institute and her students, Henry Teng, Meg Grantham, and Kevin Davis; and Andrzej Wierzbicki of the University of South Alabama.

The Laser Glass team was led by Jack Campbell of CMS in collaboration with two leading (and competing) laser glass producers, Schott Glass Technologies of Duryea, Pennsylvania, and Hoya Corporation USA of Fremont, California. This revolutionary process, the Continuous Laser Glass Melting Process, converts high-purity, powdered raw materials into one continuously moving strip of high-optical-quality laser glass. Meter-sized plates of laser glass are then cut from the end of the strip as it leaves the production system—at a rate 20 times faster and 5 times cheaper than possible with the batch process. The glass itself has 2 to 3 times better optical quality—all necessary qualifications to meet the demands of the NIF laser.

Directorate Awards

Programmatic contributions are recognized by the Program Directorates through their awards program. Awards categories for CMS are Scientific and Technical; Environment, Safety & Health (ES&H); Leadership; Operations and Administration; and Institutional Impact.

Scientific and Technical

Significant contributions to CMS in support of the weapons refurbishment program, Jacquelyn Nielsen^a

Exceptional creativity in developing new radiochemical diagnostics for old debris samples, Yves Dardenne, Jacqueline Kenneally, Nancy Stoyer^b

"Pressure Wave Measurements from Thermal Cook-off of an HMX based High Explosive" selected as best paper at the Propulsion Systems Hazards Subcommittee's Technical Steering Group, Jerry Forbes, Frank Garcia, Daniel Greenwood, Kevin Vandersall, Paul Urtiew, Craig Tarver^b

Outstanding contributions to Science Advocacy, Charles Westbrook, Nora Briant, Cindy Palmer, Lou Terminello, Trish Baisden, Jim De Yoreo, Art Nelson, Patrice Turchi, Alex Hamza, Jim Tobin, Tomas Diaz de la Rubia, John Reynolds, Joe Satcher, Randy Simpson, Alan Volpe^a First detection of plutonium aging via TEM, Wilhelm Wolfer, Adam Schwartz, Mark Wall^b

Environment, Safety & Health

Preparing the FY01 S200 Facility Self Assessments, Barbara Pulliam, Pete Baylacq, Yolanda Villa^a

Developed, tested, and rolled-out successful Facility Safety Plan (FSP) training courses, Carey Bailey, Sandra Day, Scott Dougherty, Marleen Emig, Cary Gellner, Howard Hall, Teresa Kamakea, Ken Marsh, Fred Miller, Sharon Rangitsch, Erica von Holtz, Cory Wilkinson^g



Figure 6. Laser Glass team (left to right): Paul Ehrmann, William Steele, Charles Thorsness, Michael Riley, Tayyab Suratwala, and Jack Campbell. Team members not shown: Koji Suzuki, Kohei Yamamoto, Ryo Konta, Kunio Takeuchi, and Julie Storms of Hoya Corp USA; and Steve Krenitsky, Joe Cimino, Hardy Penkratz, Michael Timms, Dave Sapak, Ed Vozenilek, Joseph Hayden, and Alfred Thorne of Schott Glass Technologies.

Leadership

Commitment to insure backup power on site when FTMS was being charged, Art Combs^b

Operations and Administration

Outstanding contributions to CMS Facts & Figures and to successfully developing "CAFÉ" (Costs, Accounts, Funding, Effort) financial database, Nancy Schoendienst^a Outstanding contributions to the Bodega Bay Workshop on Multiscale Modeling of Materials, Lisa Rose–Webb^a

Security

Extraordinary sustained effort on enhancing the effectiveness and awareness of Security, Joseph Carlson, Al Moser, Larry Newkirk, Pam Poco, Dabbie Schleich^a

Outstanding effort on enhancing the effectiveness and awareness of Security, Dawn Areson, Yves Dardenne, Howard Hall, Deborah Irish, Barbara Jackson, Jacqueline Kenneally, Marv Lima, Doug Manatt, Vicki Mason–Reed, Joanne Maxwell, Bonnie McGurn, Ken Moody, Sharon Rangitsch, Leslie Spellman, Mark Stoyer, Carol Velsko, John Wild, Nathan Wimer^a

Outstanding commitment to Security, Nathan Wimer^o

Other Awards

Charles K. Westbrook et al., received the Arch T. Colwell Merit Award for their SAE (The Engineering Society for Advancing Mobility Land Sea Air and Space International) paper entitled "Diesel Combustion: An Integrated View Combining Laser Diagnostics, Chemical Kinetics, and Empirical Validation." The paper was one of 14 selected from over 2,160 published for SAE meetings during 1999.

^aSignificant outstanding contributions beyond the scope of normal job assignments

^bExceptional creativity in the achievement of a project or assignment

^cExemplary teamwork

^dExceptional customer service well beyond normal expectations

^eExtraordinary productivity

^fAchievement of process improvements resulting in greater efficiency and/or cost savings

gExtraordinary commitment and effort to enhance ES&H awareness and effectiveness

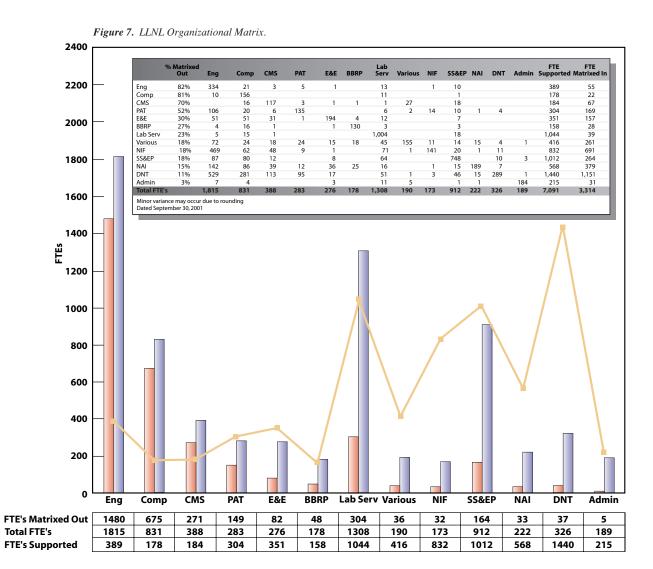
^oOther



Operations

Laboratory Programs are supported by a large technical base consisting of more than 1,000 PhD scientists and engineers. A significant portion of the scientific staff is organized into "discipline" or support directorates—CMS, Computations, Engineering, and Physics—and many of these people are matrixed, or assigned, to specific Programs. Use of the matrix system fosters

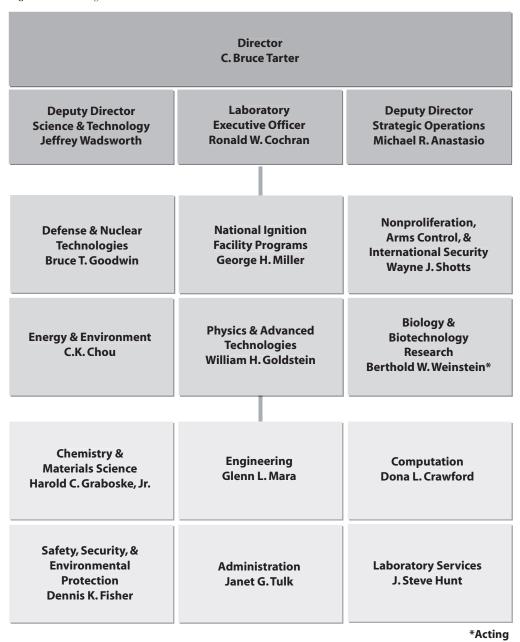
efficient transfer of technical knowledge among Programs, enables staff members to develop a wide-ranging set of skills and knowledge, and infuses projects with diverse ideas for solutions. As a result, the Laboratory has the ability to seize Program opportunities, the agility to react quickly to technical surprises, and the flexilbiy to respond to programmatic changes. The table insert in Figure 7 shows percent matrixed out along with total FTEs and the mix of FTEs supported by organization.



Organization

No standardized organizational structure exists within the Program and Support Directorates. Each Directorate is organized by its AD to more efficiently meet the needs and mission of the organization (see Figure 8).

Figure 8. LLNL Organizational Chart.



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Financial and FTE Highlights

Fiscal year ending September 30, 2001, operating and capital expenses totaled \$1,370.0M. This included \$1,088.0M for the Laboratory operating budgets and \$282.1M for capital projects. FY02 operating and capital budgets are projected to be \$1,535.0M. The staffing level as of September 30, 2001 was 7,091 full time equivalents (FTEs), including full-time, part-time, and indeterminate time employees. As of October 27, 2001, planned FTEs are 7,305. (See Table 1 for or the correct breakdown of financial and FTE information by major program.) FTEs, a term used to describe

a full-time employee who, during the course of a year, takes an average amount of vacation, sick leave, and other leave in addition to normal holiday leave. Part-time employees are counted as fractional FTEs. Therefore, FTE totals are not equivalent to number of employees.

Figures 9 and 10 show Operating costs and FTEs from FY92–01.

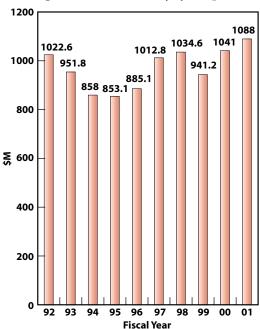
Table 1. Laboratory Costs (\$M) and FTEs by Major Program.

FY01 FY02					
	Actual 9/30/01			ned 0/27/01	
Major Program	\$(M) FTEs		\$(M)	FTEs	
Operating	(141)	1123	\$(IVI)	1123	
	277.1	1 000 7	425.1	1 241 7	
Stockpile Stewardship & Management ASCI Platforms & Alliances	377.1 73.8	1,099.7 0.0	425.1 58.1	1,241.7 0.0	
Facilities and Infrastructure	0.3	0.0	10.0	0.0	
Safeguard & Security	85.2	475.8	97.4	512.0	
Technology Transfer/CRADAs & Education	1.5	2.9	1.5	2.7	
Inertial Confinement Fusion (ICF)	31.8	98.4	43.4	124.4	
National Ignition Facility (NIF)	83.2	215.8	81.7	247.4	
Fissile Material Disposition	19.4	32.3	6.0	11.6	
Non-Proliferation & Intelligence	88.8	217.6	107.6	240.6	
Environ Restoration & Waste Mgmt (ERWN)	45.9	188.5	39.1	183.3	
Other Defense	4.2	7.5	4.5	8.1	
Fusion Energy	14.8	49.3	15.5	52.3	
Biomedical & Environmental Research	29.1	118.9	31.3	117.2	
Basic Energy Sciences	10.4	22.4	14.1	32.5	
Energy Research	8.8	25.4	30.7	30.7	
WFDOE Non-DOE	82.9	251.0	112.6	265.2	
	130.8	354.2	150.8	394.0	
Total Sponsor Funded Operating	1,088.0	3,159.7	1,229.3	3,463.7	
Capital					
DOE GPP	1.9	0.0	0.7	0.0	
DOE Line-Item Construction	28.7	42.8	48.5	11.7	
NIF Capital Construction	251.5	428.1	256.5	401.0	
Total Sponsor Funded Capital	282.1	470.9	305.7	412.7	
Total Sponsored Funded Operating & Capital	1,370.0	3,630.6	1,535.0	3,876.4	
Distributed					
Laboratory Directed R&D (LDRD)		245.4	_	234.1	
Plant Engineering Jobs	_	381.2	_	383.6	
Organization Facility (OFC)	_	292.5	_	301.9	
Organization Personnel (OPC)	_	597.1		608.8	
Program Management (PMC)	_	339.6	_	305.4	
Distributed Service Center	_	414.3	_	430.8	
Institutional General Purpose Equip	_	2.9	_	0.0	
General & Administrative (G&A)	_	1,187.3	_	1,163.8	
Total Distributed	_	3,460.3	_	3,428.4	
Total Operating, Capital & Distributed	1,370.0	7,090.9	1,535.0	7,304.8	
Minor variances may occur due to rounding					
willor variances may occur due to rounding					

Staffing and Demographics

As of September 30, 2001, the LLNL workforce (by head count) was 8,656. This workforce is comprised of 76% career, 8% term appointment, 1% postdoctoral, 8% non-career (comprised of temporary, student, faculty, retiree and miscellaneous), and 7% supplemental labor (see Table 2). The staff profile (for indefinite employees only) showed 40% scientific staff, 24% administrative and clerical, and 37% technical and crafts personnel. About 46% of the scientists and engineers have a PhD, for degree composition by job title (see Table 3). The technical discipline makes up the largest job group (26%). LLNL's scientific staff by Discipline is shown along with Postdoctoral Labor (see Table 4).





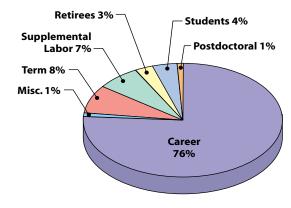


Figure 10. Ten-Year Laboratory FTEs.

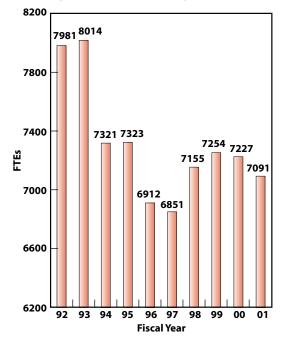


Table 2. LLNL Workforce.

Workforce Category	Heads	Staff%
Career	6,613	76%
Indefinite Full-Time	6,349	73%
Indefinite Part-Time	264	3%
Term Appointment	687	8%
Flexible Term Full-Time	655	8%
Flexible Term Part-Time	32	0%
Postdoctoral	103	1%
Postdoctoral/Grad Students	103	1%
Non-Career	687	8%
Temp	31	0%
Student/Faculty	335	4%
Retiree	263	3%
Misc.	58	1%
Total Career and Non-Career	8,090	93%
Other Labor Non-LLNL	566	7%
Supplemental Labor	566	7%
Total Laboratory Heads	8,656	100%
Minor variances may occur due to Dated: September 30, 2001	rounding	

 Table 3.
 LLNL Staff Profile by Job Title and Degree Composition.

Job Title	PhD	MS	BS	AA	No Degree	Total	Staff%
Scientists & Engineers	1,217	736	664	9	35	2,661	40%
Physicist—(270)	649	78	22	_	1	750	11%
Chemist—(242)	131	33	43	_	_	207	3%
Engineer/Patent Eng.—(168, 249)	253	365	254	4	13	889	13%
Mathematician/Computer Scientist—(256, 285)	99	204	288	4	21	616	9%
Biological Scientist—(225, 277, 235, 228, 221)	22	13	19	_	_	54	1%
Environmental Scientist—(230)	17	31	32	_	_	80	1%
Metallurgist—(265)	33	7	3	1	_	44	1%
M.D. (Staff)—(263)	5	_	_	_	_	5	0%
Political Scientist—(295)	8	5	3	_	_	16	0%
Administrative & Clerical	29	163	345	137	907	1,581	24%
Management—(196, 197)	20	60	36	5	18	139	2%
Professional—(163-165, 169, 170)	5	21	34	1	7	68	1%
Administrative—(100-162)	4	81	221	64	324	694	10%
Clerical/General Services—(400-462)	_	1	54	67	558	680	10%
Technical & Crafts	1	28	319	678	1,436	2,462	37%
Security/Fire Dept.—(051, 055, 650-656)	_	1	24	44	169	238	4%
Technical—(302-339, 393, 347-391, 502-588, 593)	1	26	281	569	865	1,742	26%
Trades—(722-799, 805-990)	_	1	14	65	396	476	7%
Facilities/OJT/Gen Helper—(700, 701, 704, 801)	_	_	_	_	6	6	0%
Total Laboratory Heads	1,247	927	1,328	824	2,378	6,704	100%
Degree Composition %	19%	14%	20%	12%	35%	100%	_
Excludes summer hires and temporary program participants Minor variances may occur due to rounding Dated: September 30, 2001							

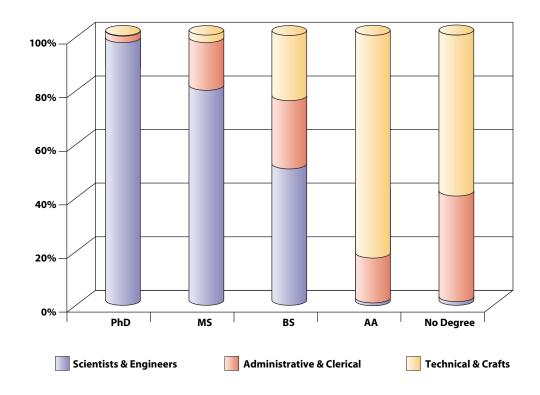
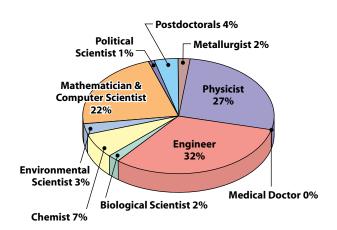


 Table 4.
 LLNL Scientists and Engineers by Discipline and Postdoctorals.

Job Title	Total	Staff%
Scientists & Engineers	2,661	96%
Physicist—(270)	750	27%
Chemist—(242)	207	7%
Engineer/Patent Eng.—(168, 249)	889	32%
Mathematician/Computer Scientist—(256, 285)	616	22%
Biological Scientist—(225, 277, 235, 228, 221)	54	2%
Environmental Scientist—(230)	80	3%
Metallurgist—(265)	44	2%
M.D. (Staff)—(263)	5	0%
Political Scientist—(295)	16	1%
Postdoctorals	103	4%
Total Laboratory Heads	2,764	100%
Includes indefinite and postdoctoral employees only Minor variances may occur due to rounding Dated: September 30, 2001		





Operations

The scientific and technical discipline activities of the Directorate can be divided into three broad categories:

- CMS staff are assigned to work directly in a Program—a matrix assignment typically involving short deadlines and critical time schedules.
- The development, management and delivery of analytical, characterization, measurement, synthesis, processing and computing capabilities and scientific services to Programs.
- Longer-term research and development activities in technologies important to Laboratory Programs, determining the focus and direction of technology-based work on programmatic needs.

Integrated Safety Management System (ISMS)

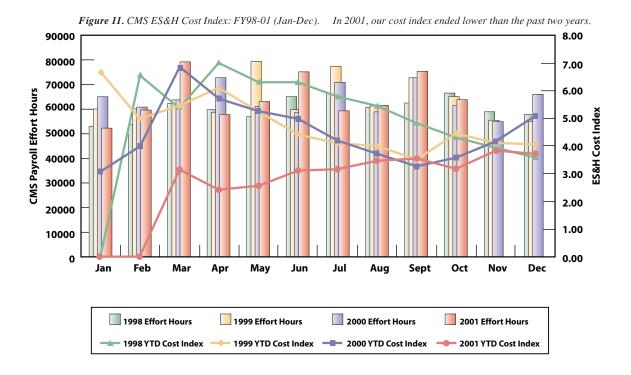
CMS applies the LLNL Integrated Safety Management System (ISMS) to incorporate quality assurance (QA) and environmental, safety, and health (ES&H) requirements into CMS research and work activities. The focus of the CMS ISMS is to provide the resources to our scientists and employees to support accomplishment of the research or work activity in a way that fulfills the ES&H requirements and to "do work safely."

To achieve the goals of Integrated Safety Management, CMS provides three safety officers and the ES&H Team 5 as support to our researchers. These resources help the researcher complete the Integration Work Sheet (IWS) process to identify ES&H requirements early in work planning. This process results in better project planning, and ultimately fewer ES&H roadblocks and better budget estimates.

Another strong component of the CMS ISMS is our Facility Safety Committees, which operate in each of the CMS-managed facilities at both Sites 200 and 300. The Committees provide one mechanism for worker involvement and resolution of safety issues affecting research and work activities in the Directorate's facilities.

While we continue to seek feedback for continuous improvement, our ISMS has helped to better define line management responsibility for work activities and increased worker involvement and awareness in safety. As a result, 95% of CMS payroll personnel believe they are safe in their workplace.

One metric of the effectiveness of the ISMS is the Department of Energy (DOE) ES&H Cost Index. The Index is a weighted score of events such as reportable injuries, lost work days, restricted workdays, and total effort hours worked. The Index allows for quick comparison of safety performance across the Laboratory and with other DOE sites. Figure 11 illustrates the general trends in performance of the CMS ISMS over the past four years.



Organization and Administration

The organization has evolved and expanded its technical breadth and depth over time focusing on a broad span of materials sciences. It now houses the institutional focus on a broad base of chemical, analytical, and the materials sciences experimental and computational expertise and capabilities. Figure 12 shows the current CMS organization. The AD office includes Infrastructure activities that span the Directorate spectrum (e.g., functions such as administration, resource management, materials program leaders, facility operations, personnel, assurances, security, and computer support). Institute activities include the Glenn T. Seaborg Institute for Transactinium Science (GTS-ITS) and the Materials Research Institute (MRI). The scientific and technical activities of the Directorate are conducted in the divisions. Organization charts are provided at the end of this publication.

The pages that follow provide summaries of the organization's key functions to include:

Infrastructure Activities

- Operations (Business/Facilities)
- Planning, Development and Personnel (PDP)
- CMS Assurance Office
- CMS Security Office

Institute Activities

- GTS-ITS
- MRI

Division Focus

- Analytical & Nuclear Chemistry (ANCD)
- Chemistry & Chemical Engineering (CChED)
- Materials Science & Technology (MSTD)

Program Focus

- Department of Defense (DoD) Technologies
- Energy and Environment (E&E)
- Nonproliferation, Arms Control, International Security (NAI)
- National Ignition Facility (NIF)
- Stockpile Stewardship Management Program (SSMP)

Capabilities Focus

- Materials Computation Analysis and Processing (MCAP) Program
- Space Action Team (SAT)

Mentoring Focus

- CMS Postdoctoral Program
- Undergraduate Summer Institute Program

Figure 12. CMS Directorate.







DNT Materials

Program Office J.N. Kass

Laser Naterials



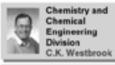




P.K. Poco



J.L. Yow







Support







Infrastructure Activities

The CMS Operations Office provides leadership and management of the infrastructure activities necessary to ensure a quality, cost-efficient workplace for the execution of scientific and technical activities. The Office manages facility, computer and business functions in support of CMS' mission (see Figure 13).



Business Operations and Resource Management— Al Moser, Operations Manager

Information Application Services

- Database development and maintenance,
- Technical writing and editing,
- Graphic design and illustration, and
- Directorate-wide Web development and maintenance.

Please see our web sites:

- cms_only: http://cmsonly.llnl.gov/
- cms_internal: http://cms.llnl.gov/
- cms_external: http://www-cms.llnl.gov/

Business Operations

Business Operations and Resource management includes the following areas:

- Budgeting (external proposals, indirect budgets);
- Cost analysis, tracking, and reporting;
- Account maintenance; and
- Audit representation and management oversight.

Procurement Services

- Managing Technical Release Representatives (TRRs);
- Processing credit card, blanket orders, requisitions;
- Providing online procurements through TRR Express;
- · Storeroom maintenance; and
- Providing access to excess equipment at federal sites.

Figure 13. CMS Operations Management Structure.





Facility Management and Maintenance— Joe Carlson, Operations Manager

Facility Operations

The management and maintenance of CMS facilities and its computer operations includes the following areas:

- Management of physical structures, building systems and facility personnel;
- Facility utilities [Laboratory Facility Charge (LFC), electricity, common use and standard telephones];
- Facility services and consumables:
 - —Industrial gases, labor support, copier rooms; and
 - Vehicles, laboratory coats, property management, and conference capabilities.
- Facility Maintenance and Improvements:
 - —CMS directed maintenance and modifications,
 - —CMS laboratory moves and reconfiguration, and
 - -Capital construction.
- Facility safety teams.

Generation of Facility Authorization Basis and Documentation

- Safety Analysis Reports (SARs), hazard analysis reports and authorization basis;
- Facility Safety Plan (FSP) generation, review and publication;
- Safety Basis Envelope and National Environmental Policy Act (NEPA)/ Environmental Impact Report (EIR) generation; and
- Emergency preparedness and response plans.

Strategic Space Planning and Utilization

- · Current and future needs of facilities,
- LLNL space and site planning interface,
- CMS program area plans (Institutional), and
- Return of facilities to the Institution.

Space Use and Utilization Processes and Leadership

- Coordination of space assignments, maintenance of tracking systems, and office move support and execution;
- Laboratory/office transfers, room responsible person (RRP) assignments, maintenance of RRP database; and
- Maintenance of billing information.

Computer Operations Desktop support and network maintenance operations

- Mac, PC, UNIX, Desktop Support;
- Network installation, connectivity and maintenance:
- Server administration;
- Printer setup and service; and
- Open Labnet connections.



Planning,
Development and
Personnel (PDP)—
Lori S. Turpin,
Deputy Associate
Director

The Planning, Development and Personnel (PDP) Office directs organizational strategic planning and implementation, including the creation, development and operation of the long-term Strategic Plan, and the implementation of organizational structural Directorate changes required by key strategies. Figure 14 shows the PDP organizational structure.

This Office is responsible for staff development for the Directorate that includes the education and training requirements for all classifications in the Directorate.

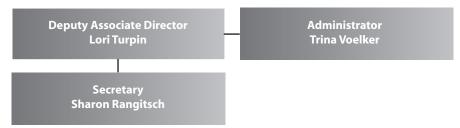
The Office is responsible for management of all Directorate personnel activities, including all aspects of the following:

- Performance management,
- Salary and compensation procedures,
- · Recruiting,
- Hiring and placement,
- Awards & Recognition programs,
- Employee Development, and
- All other personnel administrative activities.

The PDP Office is responsible for all Directorate Diversity and Affirmative Action initiatives and activities and for improving and expanding the nature and quality of communications within the Directorate.

The Office maintains appropriate knowledge of LLNL's ES&H standards, policies and procedures in identifying hazardous conditions and operations.

Figure 14. CMS PDP Organizational Structure.





CMS Assurance Office—Doug Marden, Manager

The CMS Assurance Office provides independent assurance of the implementation of ES&H requirements within CMS to its AD.

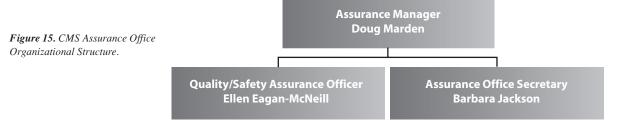
CMS ES&H Assurance

The mission of the Assurance Office is to promote a safe work place and to reduce the potential for public and personnel injury. The goals of this office are to do the following:

- Guide personnel in practices that maintain the integrity of Laboratory facilities and equipment and protect public property.
- Provide the AD with assurance that CMS operations are in compliance with applicable laws and policies.
- Favorably impact the ability of CMS Programs to meet their goals.
- Facilitate healthy and knowledgeable quality management and ES&H cultures.
- Improve the quality of ES&H programs and documents, including those developed at the institutional level.
- Encourage protection of the environment.

 These goals are pursued by the organization shown in Figure 15. Their FY01 accomplishments include the following:
- Revamped the CMS Self-Assessment Program to reduce the emphasis on formal self-assessments, instead emphasizing the importance of management and supervisor walkthroughs.
- Reviewed and commented upon revisions of the hazard analysis and safety documentation for CMS facilities.

- Completed assessments or verifications of the following:
 - Pressure Safety Systems and Relief Devices,
 - -Integrated Safety Management,
 - —Storage of Peroxidizable Chemicals,
 - —Hazards Control's Facility Safety/ Authorization database for CMS facilities.
 - —Quality Assurance,
 - —Annual Self-Assessment Report,
 - —Confined Spaces at Site 300, and the
 - —Off-site Work Reviews (Stanford Radiation Laboratory and Advanced Light Source).
- Acted as the Directorate point-of-contact for the collection and dissemination of information. Most notable of these efforts were the support provided to the following activities:
 - External audits and reviews [DOE/ National Nuclear Security Administration (NNSA), Assurance Review Office]
 - —Waste generation estimates,
 - —ES&H-related Lessons Learned,
 - National Emission Standards for Hazardous Air Pollutants accounting,
 - —Storm Water Pollution Prevention certification.
 - —Chronic Beryllium Disease Prevention Program,
 - —Self-help for LLNL Emergency Management Division,
 - —CMS Legacy materials and equipment data,
 - —CMS ES&H deficiency tracking database, and
 - —University of California (UC) ES&H Performance Measures.
- Updated Directorate ES&H documents:
 - —Directorate's Self-Assessment Plan,
 - —Quality Assurance Plan, and
 - —Visitor Safety Brochure.
- Established a Quality Management Manual website to emphasis quality assurance and management guidance.





CMS Security
Office—Pamela
Poco, Manager

The CMS Security Office facilitates, coordinates, and ensures implementations of security requirements within CMS.

CMS Security

The CMS Security Office was created in June 2000 as a coalition of personnel supporting CMS that are associated with the various aspects of security. Table 5 lists the CMS Security Office participants. The efforts of this coalition are directed toward the following tasks:

- Facilitate communication among various branches of security and CMS personnel;
- Expedite the resolution of security issues, such as the processing of paperwork for foreign nationals, followup of security infractions, and responding to DOE security initiatives:
- Ensure implementation of security-related requirements within the various CMS management chains;

- Review and recommend approval of CMS security-related documents to the AD;
- Develop tools and procedures to expedite processing of security-related paperwork within CMS; and
- Represent CMS interests on various institutional security-related committees:
 - —Computer Security Council,
 - —OpSec Committee,
 - —Sensitive Subjects Committee,
 - —Information Architecture Security Task Force, and
 - —Computer Security Working Group.

Table 5. List of CMS Security Office Participants.

CMS Security Coordinator
Classification
Computer Security
Foreign National Coordination
Personnel Security
Physical Security
Sensitive Subjects

Pam Poco Robert Hopper Joe Carlson Trina Voelker Lori Turpin Michel Dahlstrom Al Moser

Institute Activities



Glenn T. Seaborg
Institute for
Transactinium
Science (GTSITS)—Christine
Hartmann-Siantar,
Director

The Analytical and Nuclear Chemistry
Division (ANCD) is closely associated with the
Glenn T. Seaborg Institute for Transactinium
Science (GTS–ITS) whose mission is to provide
educational and research opportunities in
nuclear science at all levels, including
undergraduate, graduate and postdoctoral
appointees. The GTS–ITS seeks to develop and
enhance competencies essential to LLNL's
national security mission, by serving its
Defense, Energy and Environment, and
Bioscience and Health programs, integrating
research and education. In the spring of FY01,
Christine Hartmann–Siantar began her tenure as
Director of the Institute.

The Institute hosts an annual Actinide Sciences Summer School Program (ASSSP) in partnership with the LLNL Education Office and the Department of Energy /Defense Program (DOE/DP). The intent of the ASSSP is to encourage students to pursue scientific careers in general, and to give them exposure to the actinide sciences so that they may consider careers in these fields that are at the heart of the DOE mission. The ASSSP builds on classroom education and offers "hands-on" laboratory research work with actinides. Many of the ASSSP students have attended the American Chemical Society sponsored summer schools in radiochemistry at either Brookhaven National Laboratory or San Jose State University. In addition, during the eight-week program, the students participate in short courses presented by leading professors and scientists in the field of actinide research. Poster presentations are given by each student on his or her ASSSP research project at the end of the summer program. LLNL staff, senior management and university professors are invited to attend this poster presentation session.

During the summer of FY01, the ASSSP students participated in a variety of research projects that included:

- X-ray Absorption Spectroscopy,
- Theoretical Computational and Quantum Chemistry of Actinides,
- Modeling Migration at the Nevada Test Site (NTS),
- Column Separation of Group 14 Element (114),
- Actinide Solubility at Elevated Temperature,
- Transmission Electron Microscopy of Aged Pu,
- Rapid Analysis for Actinides by Inductively Coupled Plasma (ICP)/Mass Spectrometry,
- Migration Studies of Cs–137.

Over the past three years, 28 students have participated in the ASSSP. Some of these students have been hired into CMS as postdoctorate and technical scholars.

For further information on the GTS-ITS and the ASSSP please see our web site: http://www-cms.llnl.gov/gtsits/pages/welcome.html

Institute Activities (cont'd)



Materials Research Institute (MRI)— Michael W. McElfresh, Director

The Materials Research Institute (MRI) was chartered in March 1997 as the Laboratory's newest Institute to promote the highest quality materials research and innovation through collaboration between universities and LLNL. The Institute's goal is to enable the best university research to enhance the Laboratory's programs in the areas of cutting-edge materials science (see Figures 16 and 17).

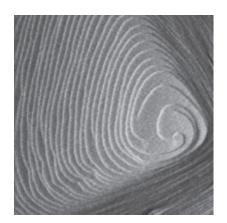


Figure 16. An 8 × 8µm scanned probe image of a source of atomic steps for growth on the face of a KDP crystal. The morphology and dynamics of crystal growth has applications to biomaterials projects within the Institute.

The Institute focuses on two primary areas of materials research:

- Nanoscience and Nanotechnology
 Novel nanofabrication methods (especially relevant to 3D mesoscopic structures), manipulation of objects/structures at the nanoscale, materials properties measured with nanoscale resolution, limits of detection, and quantum confined systems.
- Materials under extreme conditions
 Materials under conditions of high strain
 rate, high pressure, high temperature, or
 high radiation intensity. This includes laser
 material interactions, NIF materials
 experiments, fracture, equation of state,
 energetic materials, shocked materials,
 pulsed laser deposition, laser cutting, high
 pressure physics, and warm dense matter.

The MRI sponsors collaborations with universities with several programs. The UC Directed Research & Development (UCDRD) minigrants program sponsors collaborations between LLNL scientists and university collaborators. The MRI/EMC graduate fellowship program sponsors graduate students in their last few years to work on a thesis project related to an energetic materials issue jointly with a LLNL scientist and their university advisor. The summer Institute for Computational Materials Science and Chemistry brings graduate students early in their work to the Laboratory to work with a scientist on a short project with the prospect of continuing this as their thesis. A series of minicourses round out the summer program. In addition to these programs, the MRI participates in other LLNL student programs and works to pair university collaborators with LLNL scientists.

Figure 17. A group of KDP crystals grown at LLNL within the Laser Program. The MRI is coordinating efforts at several leading universities in using advanced spectroscopic techniques to study the fundamental processes leading to laser induced damage in these materials.



Division Focus



Analytical & Nuclear Chemistry Division (ANCD)—Judy Kammeraad, Division Leader

The primary mission of the Analytical and Nuclear Chemistry Division (ANCD) is to support scientific and technical problem solving in the national security interest. This work is conducted in a number of programmatic mission areas that are central to the Laboratory. Currently, ANCD staff support the following programs:

- Defense and Nuclear Technologies (DNT), including the Stockpile Stewardship Program;
- Nonproliferation, Arms Control, and International Security (NAI);
- National Ignition Facility (NIF) Program; and
- Energy and Environment, and Environmental Protection Department programs.

In addition, ANCD personnel work closely with the GTS-ITS and the BioSecurity Support Laboratory on a wide variety of bio-related research activities for National Security and Health. Our work in this area is performed in collaboration with scientists in other organizations, including Biology & Biotechnology Research Program, and NAI, as well as external organizations such as UC—Davis and UC—San Francisco.

ANCD possesses a suite of scientific capabilities that are exercised to support programmatic problem solving as well as fundamental research and development. These include the following:

- Bioanalytical Mass Spectrometry,
- Computational Biochemistry,
- Inorganic Analytical Chemistry,
- Inorganic Mass Spectrometry,
- Isotope Geochemistry,
- Organic Analytical Chemistry,
- Nuclear Radiation Detection and Spectroscopy,
- Nuclear Properties of Actinides, and
- Radiochemistry.

ANCD scientific capabilities encompass a very wide suite of techniques that are practiced at state-of-the-art levels. Competitive institutional investment is available to insure that world-class research opportunities can be aggressively pursued, thereby assuring the scientific health of the practicing disciplines. Recent institutional investments have provided ANCD scientists the best commercially available instrumentation in several areas. These include: Fourier Transform Ion Cyclotron Resonance Mass Spectrometry, Glow Discharge Mass Spectrometry, Nuclear Magnetic Resonance, ICP Magnetic Sector Multicollector Mass Spectrometry, and Matrix-Assisted Laser Desorption Ionization Mass Spectrometry. In the near future, a Secondary Ionization Mass Spectrometer with the best commercially available spatial resolution (50 nm), known as a "Nano-SIMS", will be installed, allowing isotopic and elemental studies at the sub-cellular scale for biological studies as well as high-resolution material composition and structure studies. These capabilities join many existing analytical capabilities, including noble-gas mass spectrometry, radiochemical separations, and nuclear radiation counting. Our gamma-ray spectrometry analysis codes are utilized in many national security programs as well as environmental programs. One such code, MGA, is used by the IAEA and Euratom and is internationally accepted as the standard for the analysis of plutonium isotopics.

Certified analyses on a wide variety of unknown samples of an environmental nature, including mixed waste, are performed routinely by the CMS Environmental Services (CES) laboratories in ANCD. This service is provided to the institution and to other DOE sites, and represents one of the best such capabilities in the DOE Complex (see Figures 18a and b).

In addition to performing applied research in support of LLNL programs, ANCD scientists participate in fundamental research in several areas including plutonium science, heavy element research, non-covalent interactions between biomolecules, transport of actinide colloidal complexes in groundwater, and isotopically enhanced molecular targeting. Of particular note, the heavy element research group in ANCD has been active for decades in the search for stable superheavy elements,

which are predicted to exist near atomic number 114 (neutron number 184). A collaboration of the LLNL group with scientists at the Joint Institute for Nuclear Research in Dubna, Russia, has recently published the discovery of new superheavy elements. In 1999 they reported the synthesis of element 114, and in 2000 they reported the synthesis of element 116. This ongoing research exemplifies excellence in scientific accomplishment in ANCD and at LLNL (see Figure 19).



Figure 18(a). CES employs state-of-the-art chemical analytical equipment and nuclear counting instrumentation to conduct its major mission of providing reliable analytical data on LLNL wastewater, other liquid waste and solid waste as part of LLNL's compliance with federal, state, regional and local environmental requirements. For example, CES employs a Dionex DX500 Ion Chromatograph fitted with autosampler for the determination of low-level concentrations of anions in water samples.



Figure 18(b). CES chemist performs complex analytical procedures to identify and quantify contaminants in environmental and hazardous/mixed waste samples in support of DOE's environmental protection and monitoring, waste management and remediation programs. CES provides certified and non-certified, rapid, high-quality chemical and radiochemical characterization on a variety of sample materials tailored to the needs of its customers.



Figure 19. Joint Livermore–Dubna team in front of the gas-filled-recoil separator.

Division Focus (cont'd)



Chemistry & Chemical Engineering (CChED)—Charles Westbrook, Division Leader

The Chemistry and Chemical Engineering Division (CChED) has a primary mission to support the major Laboratory missions. To accomplish this and to be recognized by the scientific community at large, five scientific disciplines have been identified and are being utilized to foster growth in science and technology. Each discipline has a leader who is responsible for the growth and development of that capability, in both the programmatic and technical areas. Key activities and important recent accomplishments in each discipline are summarized as follows:

Chemical Engineering is a fully matrixed capability with staff involved in a number of high profile projects, including optics development for the NIF, high explosives and energetic materials development for the Stockpile Stewardship Program (SSP) in the DNT directorate, and assessments of foreign threat assessments and capabilities for development of weapons of mass destruction in the NAI directorate. Specific highlights include the following: NIF Program Support—the development of techniques to mitigate etch pitting on NIF optical surfaces, other strategies to reduce defects in optics resulting from manufacturing and processing, and significant improvements in production of diffractive optics (see Figure 20). CChED's chemical engineers provide leadership in the following positions: the Laser Materials and Optics Technology (LMOT) Program, final optics assembly for NIF, KDP (potassium dihydrogen phosphate) Optics Cleaning and Coating, and the Diffractive Optics Group.

Energetic Materials Program Support—commissioning and licensing of a new type of molten salt unit for destruction of waste high explosives for the Republic of Korea, development of alternative new methods for destruction of unstable and excess munitions, and continued development of improvements in high-explosive technologies. CChED's chemical engineers provide leadership in the following key positions: Program Element Leader and High Explosive Focus Area Leader, the Demilitarization Program Leader and the Project Leader for the LLNL Molten Salt Oxidation Program.

Counterproliferation Analysis and Planning System (CAPS) program in NAI—CChED's chemical engineers are major participants in the efforts to evaluate capabilities of foreign organizations to produce weapons of mass destruction by analyzing their resources and industrial capabilities.

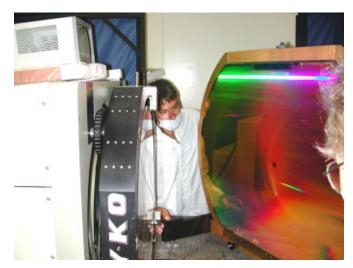


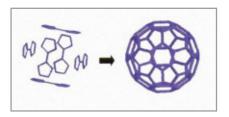
Figure 20. A 94-cm diameter diffraction grating produced by our Diffractive Optics Group.

Computational Chemistry is a central part of the research portfolio in CMS. Computational chemistry of energetic materials is investigating detonation and slow combustion of explosives, kinetics of high energy density materials, and electronic structure modeling for high explosives. Combustion chemistry in CChED deals primarily with model simulations of ignition, flame propagation, quenching and emissions from internal combustion engines. Reaction mechanisms have been developed to study the influence of fuel molecular structure on ignition properties such as octane and cetane ratings of automotive fuels. Computational chemistry of heavy elements uses relativistic electronic structure techniques to study actinide element chemistry. Chemical warfare agent modeling is developing kinetic models for surrogate and actual CW agent chemicals for use in a variety of atmospheric dispersion and other accident and terrorist scenarios. Specific highlights include the following:

Computational Chemistry of Energetic Materials—the use of electronic structure techniques to propose a novel energetic material consisting of a nitrogen analog N₆₀ of the familiar carbon buckyball, as shown in Figure 21; although only metastable, this compound would provide enormous energy storage capabilities. Continued development of computational tools to model reactive flow in energetic materials led to a new edition of the internationally used Cheetah code.

Combustion Chemistry—simulations of a new way to understand diesel engine combustion from ignition through soot formation and burnout. Related chemical kinetic research demonstrated how oxygen-

Figure 21. Schematic for constructing a N₆₀ buckyball from smaller nitrogen compounds.



ated hydrocarbon fuels reduce soot emissions from diesel engines and how a few particularly important gas phase chemical reactions control most ignition phenomena including detonations and engine knock. A collaboration under a CRADA with Cummins Engine Co. developed and demonstrated the central role played by gas phase chemical kinetics in the new automotive engine concept named Homogeneous Charge, Compression Ignition, which shows great promise for enhanced combustion efficiency and drastically reduced pollutant emissions.

Computational Chemistry of CW Agents—has led to the development of kinetic models for a number of frequently used surrogate compounds to simulate the reaction of the actual chemical warfare (CW) agent Sarin. A detailed kinetic model for Sarin was developed for the first time, and model comparisons between the chemistry of Sarin and its surrogates improved our ability to simulate CW phenomena.

- Energetic Materials represents a key scientific, as well as a programmatic activity for CChED. Besides the aforementioned computational chemistry efforts, activities in Energetic Materials include performance and aging testing, materials characterization (chemical, mechanical properties, thermodynamics, and equation of state), and synthetic organic chemistry. The Energetic Materials Center (EMC) is a world-class experimental facility that is a unique cornerstone of CChED. In addition to the EMC, the Energetic Materials Program maintains a considerable range of facilities and experimental activities at Site 300, where large-scale experiments and synthesis of explosives are conducted.
- produces novel materials for a wide range of programmatic efforts. The most highly developed capability consists of the sol-gel and aerogel research and technology that has been producing coating materials for NIF optics and ultra-low density materials for DNT and other programs for some years. An important new development has generalized the synthesis technique for low-density materials so that aerogels and other

ultra-low density materials can now be synthesized incorporating almost every element in the periodic table, rather than the four or five elements previously available, thus increasing the flexibility and variety of applications of such materials.

Another new project with significant new accomplishments consists of the development of a new glucose sensor for use in miniaturized implanted diagnostic and treatment methodologies. This work, performed under a CRADA with Medtronic/Minimed, received a DOE Bright Light Award as well as a Federal Laboratory Consortium Award this year for its accomplishments and promise for the future.

New projects in chemical synthesis involve development of new molecules with exciting potential applications as microscopic biosensors, dendritic structures for development of new polymer systems, and functionalized thiacrown ethers for waste water remediation. Other projects are directed towards synthesis of new molecules for studies of material aging and other unique nanomaterials.

Other novel developments are intended to combine unique CChED capabilities in chemical synthesis with programmatic needs of key program collaborators. A new example is the coupling of aerogel technology with the key scientific capabilities of energetic materials, leading to the development of energetic nanomaterials with variable compositions that can provide variable and programmable energy release. Figure 22 shows an example of this type of sol-gel derived pyrotechnic material. This type of collaboration may have enormous impacts on the future of energetic materials for almost limitless applications.

Physical Chemistry has historically built a
base of fundamental understanding of
materials compatibility and chemistries
through chemical optical spectroscopy.
Key capabilities also include laser-induced
chemistry and general photo-chemistry,
data processing, molecular dynamics and
kinetics. CChED physical chemists
contribute to weapon materials compatibility and aging studies, analysis and testing of

energetic materials, studies of NIF optics damage mechanisms and Inertial Confinement Fusion (ICF) and NIF target design and production, and to applied spectroscopy for NAI's programs. Similar to the chemical engineering capability, physical chemistry is also a fully matrixed workforce that provides research and leadership for a widerange of Laboratory efforts.

The growth of these scientific capabilities is directly related to long-range programmatic needs and to facilitating the growth of new strategic opportunities. CChED will continue to improve its collaborations with Laboratory programs and to initiate scientific and technical capabilities for their future needs.



Figure 22. Test of a sol-gel based pyrotechnic device.

Division Focus (cont'd)



Materials Science & Technology Division—Lou Terminello, Division Leader

The Materials Science and Technology Division (MSTD) is a Division of about 135 scientists (75%) and scientific support (25%) personnel. It is organized into a number of program elements and scientific capabilities a hybrid of program and discipline focus that reflects the numerous ways it serves the materials science needs of the Laboratory. Program elements are aligned with specific projects in DNT, Energy and Environment, NIF, and NAI. In general, MSTD is focused on metallurgy, electrochemical processing, materials science, material characterization, surface science, solid-state chemistry, and materials theory and modeling. Its workforce is comprised of chemists, physicists, metallurgists, ceramicists, chemical engineers, materials scientists, and mechanical, chemical, and electrical technicians. This professional diversity and broad subject matter expertise makes MSTD a valuable component of an evolving Laboratory.

MSTD maintains expertise in the characterization and modeling of the mechanical properties of metals and in the development of relationships between microstructure and properties. This also includes experience with the mechanical properties of inorganic composite materials as well. The joining element spans the entire range of metallic and non-metallic inorganic materials joining. Joining of exotic, toxic or hazardous materials is a specialty. MSTD also maintains a well-equipped metallography laboratory that serves the needs of many programs.

Its metals processing capability has the ability to synthesize and process metals in a number of different ways. In metals processing, we can melt and cast experimental alloy compositions using vacuum induction melting and electron beam cold hearth melting; small quantities of material can be alloyed using an electron beam button melting furnace; material can be hot forged and hot

and cold rolled; swaging and cold drawing are possible to provide wire and rod sample materials; materials can be shaped by hot forming, deep drawing and spin forming. Vacuum, inert gas and ambient heat treating capabilities are available to further control the physical properties of materials processed by the variety of hot and cold working processes. Room temperature and high temperature testing capabilities are available to characterize the physical properties of the test material.

Both chemical vapor deposition (CVD) and physical vapor deposition (PVD) facilities are available to fabricate shapes or provide surface coatings. These processes can provide shapes in hard to fabricate materials such as tungsten or provide surface coatings useful in providing corrosion, oxidation and wear resistant surfaces. We have a world-recognized capability in multilayer fabrication for x-ray optics and other applications. A recent accomplishment of this program was development of the optics for the TRACE x-ray telescope. Solar x-ray images captured with these optics are shown in Figure 23.

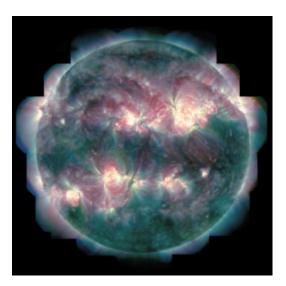


Figure 23. Image of the Sun overlaying various temperatures—color overlay: 1MK (green), 1.5 MK (blue), 2 MK (red).

The electrochemistry capability can provide innovative solutions to a variety of problems, such as innovative battery concepts, waste treatment, refinement and extraction of metal from salts, a wide variety of electrochemical sensors, and the use of the bipolar cell for lithium metal recovery from lithium chloride. The development and study of corrosion technology uses MSTD's electrochemistry capability. Proper design of hardware and structures requires the understanding of the corrosion of materials, sometimes on a geological time scale as in the Yucca Mountain Program. Testing facilities are available to help assess and predict corrosion behavior.

A full suite of materials characterization capabilities is available, i.e., scanning electron microscopy, Auger spectroscopy, Rutherford backscattering and associated techniques using our 4 MeV ion accelerator, x-ray diffraction, atomic force microscopy, scanning tunneling microscopy, and various synchrotron based analytical methods. The state-of-the-art transmission electron microscope (TEM) was obtained jointly by CMS and DNT. We have fully instrumented, experimental surface science capability to carry out sample preparation, modification, characterization, including in-situ analytical measurements

during transient behavior. Recent accomplishments of the materials characterization capabilities include detailed materials investigations for NIF laser optics and DNT stockpile materials (see Figure 24). A precision bonding facility allows detailed investigation of interfaces between a wide range of materials. These capabilities support the dual mission of fundamental research and direct support of Laboratory programs. One example of the fundamental research produced by these capabilities lies in the nanoscience and technology areas of crystal growth, quantum confinement, and bioinorganic interfaces.

MSTD has a world-class materials theory and modeling capability to calculate materials structure and properties over many length scales from quantum mechanics (total energies, magnetic, electronic, thermodynamic and transport properties), atomistic simulation applied to defects and diffusion in solids (radiation damage, ion implantation, dopant diffusion), phenomenalogical modeling of processes (metal working operations such as casting, welding, material failure such as crack propagation, fatigue) and other theoretical work. Our material modeling and theory capability is an essential tool for the Laboratory's programs and for our basic and applied research (see Figure 25).

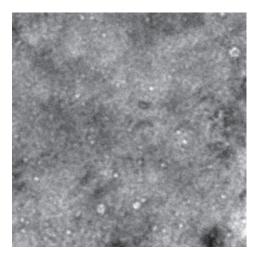


Figure 24. Micrograph showing helium bubbles in 35 year old Pu.

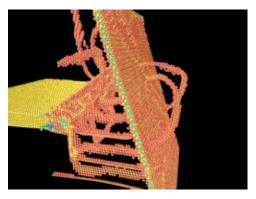


Figure 25. 100-million atom simulation of interacting crack, dislocations and grain boundary.

Program Focus



Department of
Defense (DoD)
Technologies—César
O. Pruneda,
Materials Program
Leader

The objective of this office is to expand the CMS Directorate's portfolio of DoD projects and to coordinate non-DoD work-for-other (WFO) activities. The science and technology applied in the DoD and WFO projects serve to enhance and build CMS competencies that support Laboratory Programs in national security, energy and environment, and bioscience and healthcare. These Program development activities are performed and managed solely by CMS or collaboratively with other directorates and LLNL's DoD Programs Office. Another outcome of CMS DoD and WFO activities will be opportunities to develop and enhance the project leadership and management skills of CMS personnel.

The DoD Materials Technologies Leader Team includes CMS Division Leaders, Materials Program Leaders (MPLs), and key program element personnel.

CMS' current DoD and WFO portfolio is varied both in the level of funding of individual projects and range of sponsoring agencies, private and governmental. Current DoD Technologies Office priorities include expanding programs in:

- Energetic materials synthesis, formulation, manufacturing, performance, vulnerability, reliability, storage, and demilitarization.
- All areas of chemical warfare/biological warfare (CW/BW): signatures, detection, analysis, mitigation, and demilitarization; activities in this arena will focus on identifying and engaging appropriate DoD elements collaboratively with CMS NAI MPL and NAI personnel.
- DoD environmental arenas where CMS and Energy and Environment directorates (and others) have unique capabilities that can be coupled collaboratively to address pressing national needs in these areas; activities in this arena are performed collaboratively with CMS Energy and Environment MPL (Jesse Yow) and personnel from other directorates.

Other priorities include working with the relevant CMS MPLs in identifying strategic directions and investments that can make an impact on DoD and WFO program development activities.



Energy &
Environment
(E&E)—Jesse Yow,
Materials Program
Leader

The CMS Energy and Environment Materials Program Office (MPO) supports programs conducted by the Energy and Environment (E&E) Directorate and Environmental Protection Department at LLNL. These programs work in three highly cross-linked and multidisciplinary areas at the intersection of U.S. energy, environment, and national security interests:

- Nuclear Materials and Systems, including:
 - Repository systems for nuclear waste disposition;
 - Nuclear fuel cycle materials and technologies;
 - —Complex engineered materials performance and simulation;
 - Advanced systems for nuclear energy and proliferation resistant fuel cycles; and
 - —Nuclear systems safety and security.
- Energy/Carbon/Climate, including:
 - —Carbon utilization, separation, capture, and sequestration;
 - —Energy conversion, storage, and use;
 - —Fuel system and fuel additive modeling and assessment:
 - —Combustion kinetics and modeling;
 - -Advanced and durable materials.
- Environmental Security, including:
 - —Environmental monitoring and assessment;
 - —Remediation and waste management technologies;
 - Energy and environmental infrastructure protection;
 - Water resource characterization and diagnostics; and
 - —Multiscale (temporal and physical) atmospheric fate and transport.

CMS provides energy and environmental programs with about 40 FTEs of direct and indirect support, with people working in program and project leadership as well as technical support assignments. About 20 additional FTEs support

these programs through recharged analytical services. The programs benefit from several LDRD projects that support energy and environmental interests:

- Resolving nuclear reactor lifetime extension questions: a combined multiscale modeling and positron characterization approach;
- The dependence of reactivity of carbon electrochemical fuels on structure; and
- Colloidal transport of actinides in the vadose zone.

Jesse Yow leads the CMS Energy and Environment MPO Team (see Table 6) that supports energy and environmental programs by:

- Providing a direct interface between the energy and environmental programs and CMS:
- Assisting energy and environmental organizations with strategic planning, new initiatives, and scientific review;
- Coordinating scientific and technical staffing for responsive support;
- Facilitating program access to CMS capabilities and facilities; and
- Coordinating research and technology development to anticipate and meet program needs

FY02 program development activities will focus on nuclear fuel cycle research and closure, carbon fuel cycle and greenhouse gas management, energy storage and conversion technologies, atmospheric fate and transport, environmental security, environmental risk characterization and mitigation, and other areas determined by program investment strategies.

Table 6. E&E MPO Team members (others are added as needed).

E&E Materials Program Leader	Jesse Yow
Team Members	Bryan Bandong John Cooper Nerine Cherepy Brad Esser Alan Jankowski Annie Kersting Mukul Kumar Cindy Palmer Quoc Pham Bill Pitz Dave Smith Steve Steward Tammy Summers Brian Wirth



Nonproliferation, Arms Control, and International Security (NAI)— César O. Pruneda, Materials Program Leader

The NAI Directorate's mission is to support the U.S. government and international agencies in their efforts to reduce the danger from nuclear weapons and other threats from weapons of mass destruction.

The NAI MPO objective is to promote the success of NAI programs by facilitating NAI—CMS interactions, providing technical experts, coordinating collaborative research, assisting in program development, and building or enhancing key CMS capabilities.

Materials Program Liaison, César Pruneda, NAI MPO team [and interface] members are shown below in Table 7.

The total for CMS effort in NAI programs is approximately 40 FTEs of which about 30 are essentially full time in the NAI program elements:

- Forensic Sciences and other R-Division programs,
- Proliferation Prevention and Arms Control, and
- Counterproliferation Analysis and other Q-Division programs.

Current MPO priorities include the following:

- Identify areas for cooperative CW/BW program growth; team with key experts in NAI, Biology and Biotechnology Research Program (BBRP), Earth and Environmental Sciences (now part of Earth and Environment Directorate), and other directorates to pursue selected opportunities.
- Promote joint Laboratory Directed Research and Development (LDRD) projects in NAI-related research.
- Undertake the development of selected capabilities ("technology development") that aid NAI and other programs.
- Promote strategic investment of Institutional General Purposed Equipment (IGPE) funds to build CMS capabilities that aid NAI and other programs.
- Assist NAI in finding excellent chemical engineers for the Counterproliferation Analysis and Planning System (CAPS) program.
- Help NAI link and promote LLNL radiation detection experts and capabilities to benefit all of the programmatic and discipline stakeholders.
- Continue to aid the Forensic Science
 Center by providing technical experts,
 managing the matrix environment
 effectively, and promoting the
 enhancement of key technical capabilities.

Table 7. NAI MPO Team (and interface) members.

NAI Materials Program Leader
Q & Z Divisions, PEL
Forensic Science Center, PEL
Radiation Detection Center
PPAC, PEL
Team Members

August Droege Pat Grant Judy Kammeraad Wayne Ruhter Chuck Stevens Dave Shoemaker Martyn Adamson Bill Wilson

César Pruneda



National Ignition Facility (NIF) Program— Tomas Diaz de la Rubia, Materials Program Leader

The NIF will produce conditions where nuclear fusion reactions may be studied and materials tested at extreme temperatures and pressures. The CMS Directorate provides the NIF Programs Directorate with about 50 FTEs of assigned matrix support. The NIF Materials Program Office has three strategic focus areas, namely (1) Optical and non-optical materials for the NIF laser; (2) Target R&D and fabrication for ignition and weapons physics studies, and (3) Materials dynamics at extreme conditions.

About 40 chemists, physicists, materials scientists, and chemical engineers in CMS work in an integrated fashion to develop and field optical materials for high peak power lasers, as well as to evaluate and solve non-optical materials performance issues. Another 5 FTEs work in the NIF target R&D area developing novel materials fabrication and assembly technologies to meet ignition requirements and the mission needs of the Stockpile Stewardship program. CMS scientists are also bringing their expertise in experimental and computational materials science to complement the work of NIF Programs Directorate physicists in the area of high power laser-driven materials dynamics.

Some examples include:

- Continuous melting technology for laser glass,
- Rapid crystal growth technology for KDP (see Figure 26).
- High-speed, deterministic polishing of fused silica lenses and windows,
- Diffractive optics fabrication for beam uniformity and color separation (see Figure 27),
- Fabrication of inertial fusion targets in support of energy research and defense programs,
- Precision cleaning and anti-reflection coatings for optical components,
- Design and characterization of experiments to understand laser-driven shock dynamics and microstructure evolution in metals, and
- Complementary multiscale modeling and simulation of shock driven dynamics experiments in metals.

The CMS Directorate provides resources for technology development activities that benefit multiple programs. These science and technology projects are intended to provide benefits that enhance CMS' ability to be responsive to the needs of the Laboratory as a whole and enhance the value of CMS' disciplinary staff to the programs. In addition, the NIF Materials Program Office develops and coordinates a range of LDRD projects focused on the science of laser-materials interaction, target design and fabrication R&D.



Figure 26. Rapid crystal growth technology produces large potassium phosphate crystals.



Figure 27. Chemical engineer inspects a diffraction grating.

Stockpile Stewardship Management Program (SSMP)— Jeffrey Kass, CMS Materials Program Leader

CMS supports many of the Stockpile Stewardship tasks and programs conducted by the DNT Directorate. These tasks and programs enhance U.S. defense capabilities through innovative materials and chemical R&D and the application of new science and technology to issues of concern to the U.S. Defense community. CMS assists all DNT organizations with strategic planning efforts as required, new program initiatives, and scientific reviews.

Program representatives are shown below in Table 8. The goals of the Office are extensive, including, but not limited to, the following:

- Provision of oversight and coordination for all CMS support to Stockpile Stewardship (A, B, and W programs).
- Provision of the highest quality staffing and technical training for programmatic work
- Planning and execution of R&D required for programmatic success.
- Assistance in identifying and providing required capital equipment.

that laboratory and experimental activities are cost-effective and high-quality, providing suitable input to allow proper CMS staff administration and facilitation of effective two-way communications of program goals, issues, and progress.

CMS provides DNT programs with over

Keys in achieving these goals are assurance

CMS provides DNT programs with over 100 FTEs of assigned matrix support. The Nuclear Component Materials and Chemistry funding, Tech Base funding and LDRD tasks provide direct program support, reduction to practice and forward-looking research, respectively. Due in large part to the growth of the overall funding level, the SSMP office has strengthened the coordination of CMS work internally as well as facilitated better communications. It has moved top people into crucial DNT assignments in HE, compatibility, Pu metallurgy, surveillance and radiochemistry. Actinide analytical chemistry has recently been strengthened by the assignment of high quality staff and management.

Five focus areas of intense investigation under the Nuclear Component Materials and Chemistry umbrella that will continue to be investigated in FY02 are:

- Compatibility efforts,
- Direct system support,
- Accelerated aging efforts for Pu,
- Radiochemistry assessments/actinide analytical chemistry, and
- HE safety/properties/retention of synthesis capability.

FY02 Technology Development projects related to SSMP interests include:

- Pu shock physics, and
- · radiochemistry.

Under the auspices of LDRD, the SSMP Office will:

- Investigate aging effects and defect structures in Pu,
- Experimentally validate theoretical interatomic potentials,
- Map enhanced nuclear stability in the heaviest elements,
- Investigate microstructure orientation effects on properties,
- Apply molecular dynamic calculations to HE safety, and
- Apply aerogel technology and synthesize new nanostructure HEs.

Table 8. SSMP MPO Team members.

SSMP Materials Program Leader **Jeffrey Kass B-Program Rep Elaine Chandler A-Program Rep Dave Stanfel** W-Program Rep **Ron Streit** CMS Participants: **Deputy MPL** Jim LeMay Pu/U and B-Program **Gil Gallegos** Pu and W Program **Bart Ebbinghaus** Compatibility **Bill McLean Bill Wolfer** Modeling **Radchem & Analytical Chemistry Ken Moody** ΗE Jon Maienschein HE **Randy Simpson**

Capabilities Focus

Materials Computation, Analysis and Processing (MCAP) Program

The MCAP mission is to nurture CMS core capabilities to solve key LLNL materials problems. As its primary responsibility, MCAP strategically manages and invests in CMS scientific capabilities to sustain and enhance their value to the Laboratory's mission and programs. In addition, MCAP is responsible for guiding capabilities through the stages of their life-cycle development, including standardization of techniques and processes, use by customers, and revitalization or demise. MCAP was implemented in FY98 as CMS' Strategic New Initiative.



IGPE and Recharge— Howard Hall

IGPE and Recharge

Major FY01 Accomplishments

- Managed \$2.1M of IGPE investment in CMS capabilities.
- Incorporated recharge laboratories into the MCAP Service Center (\$6M).
- Realigned specific recharge laboratories to allow better cost recovery and better alignment with customer needs. Customers recharged instrumentation time and received direct labor charges from analysts.
- Supported the activities needed for the startup of Fourier Transform Mass Spectrometer (FTMS) laboratory and the aerosol Time-of-Flight (TOF) MS capability.

FY01 IGPE Investments

- FTMS,
- TwinSNOM: Twin scanning near-field optical microscope, and
- TOF secondary ion MS.

FY01 Strategic Actions

- Continue improving MCAP business practices,
- Continue to focus on meeting multiprogrammatic demands by providing critical materials technologies, and
- Continue developing formalized MCAP investment strategies that map onto CMS strategic vision.

MCAP Investment Initiative Areas



Biosecurity and Support Laboratory (BSSL)—William D. Wilson

BSSL—the goal is to provide the scientific infrastructure and expertise necessary for LLNL to support multidisciplinary biosecurity efforts across the laboratory. The initial phase of the BSSL startup was completed in 2001. Plans for FY02 include determining and implementing the most effective mix of capabilities needed to detect, identify and characterize toxins and pathogens.



Radiochemistry— Christine Hartmann–Siantar

Radiochemistry—the goal is to further develop and implement strategies to establish capabilities for imaging and detecting gamma radiation based on existing technologies. Potential applications to a variety of LLNL programs can be envisioned, however the emphasis lies on applications for medical diagnostics and therapy. The capabilities developed within this project will be applicable to a number of Laboratory programs.



Computational
Chemistry—Andrew
Quong

Computational Chemistry—the goal is to establish a capability in multiscale modeling of biological processes. This project will benefit DNT, E&E, NAI, and BBRP as it adds a new capability and user base to ALE3D through the development of a new cell modeling capability.

Capabilities Focus (cont'd)



Space Action Team (SAT)—Mitch Waterman, Program Leader

The Space Action Team (SAT) is an integrated multi-disciplinary, multi-directorate, cross-trained team with diverse talents and skills dedicated to safely, economically, and efficiently plan and execute facility projects to support Laboratory missions. The team's functional capabilities comprise facility, project, and assurance management staff coupled with Hazardous Waste Management (HWM), ES&H technicians, and craft support, teamed with professional ES&H disciplines. SAT has two primary objectives:

- to work in partnership with its customers to support facility-related issues and concerns that impact client research activities.
- to manage the Laboratory's surplus and/or excess facilities transition process into a low-cost, safe configuration.

If a facility's disposition is determined as end-of-life cycle, the SAT designs and executes the decommissioning, deactivation, decontamination and demolition (D&D) process. SAT uses a cradle-to-grave process to achieve this, working hand-in-hand with its customers to define and execute their projects.

The team's staffing configuration is designed to implement moderate- to high-risk facility projects.

SAT, based in the CMS Directorate, operates as a service organization and supports clients throughout the Laboratory. SAT's methodology is outlined in two site-wide Operating Safety Procedures (OSPs) developed specifically for the team's unique operations and missions.

FY95-00 Projects

- D&D of perchloric/beryllium/rad contaminated exhaust systems;
- Deactivated 23 surplus and/or standby research buildings (pending disposition) into a low-cost, safe configuration;
- D&D of 15 Laboratory surplused R&D real property facilities;
- Planned and executed over 260 programmatic research relocation and/or disposal activities (e.g., wet chemistry labs, physics labs, surplus low-level waste); and
- Supported division-level organizations in their migration to jointly accomplish the following:
 - —co-locate functional groups to enhance collaborative research activities,
 - lower operating costs and enhance facility capabilities,
 - —coordinate more efficient use of space, and
 - —release and dispose of nonessential surplus contaminated equipment and property.

FY01 Projects

- D&D of Building 227 (~8400 ft²) (see Figure 28),
- Decontaminate a Lawrence Berkeley National Laboratory facility of beryllium, lead, and asbestos;
- Neutralize and dispose of a leaking Ref6 cylinder;
- Initiate the deactivation of the AVLIS facility (Building 177);
- Transfer and D&D of 13 small excess structures/trailers; and
- Deactivate 23 surplus and/or standby research buildings (pending disposition) into a low-cost, safe configuration.

FY02 Planned Projects

- D&D of Building 222, south wing (~22K ft²),
- D&D of 3 small excess program facilities,
- Complete deactivation of the AVLIS facility, Building 177 (~16K ft²),
- Initiate the deactivation of the AVLIS separator,
- Assess assets for value salvage sale of surplus/excess facility/research equipment, and
- Remove HEPA filters site-wide to support the Laboratory's HEPA upgrade project.

Figure 28. Building 227, a wet chemistry surplus facility, used to support weapons research activities.

(a) Before



(b) After



Mentoring Focus



CMS Postdoctoral Program—Glenn Fox, Program Leader

The CMS Postdoctoral Program gives the postdoctoral associates a broad and career enhancing experience, exposing them to a wide variety of research, facilities, and scientific staff. Historically, postdocs have had a difficult time integrating into the Laboratory's unique culture. Therefore, the Postdoctoral Program provides a resource for information, needs, and guidance in how to effectively navigate at LLNL. Tools that enhance the program include:

- New Employee Orientation
 (Quarterly)—This presentation provides
 an overview of the history of LLNL, the
 role of its Programs, CMS, safety, security,
 and other informational resources useful for
 day-to-day activities. The presentation is
 also available on the internal CMS website.
- Postdoctoral Symposium—A series of talks and poster sessions given by the postdocs to highlight their research activities and capabilities.
- Postdoctoral Social Events (Quarterly)—
 The postdocs, mentors, and management meet during lunch to hear a guest speaker and to discuss concerns and current Laboratory and scientific events.
- Monthly Postdoctorate Seminars—The Program strongly emphasizes educating the postdoctorate staff about other programs and science around LLNL. The monthly seminar provides a variety of speakers (all CMS postdocs are required to present at least once during their tenure).

- LLNL has research facilities and resources virtually unique to any other laboratory in the country. The Postdoctoral Program is facilitating interactions between CMS postdocs and these capabilities, providing points of contact and other needed information.
- Portfolio—The Postdoctoral Program hires research associates in identified strategic CMS research areas to include: bio-mass spectroscopy, computational chemistry, and synthesis chemistry. Since postdocs are becoming better integrated into scientific and programmatic projects, several of them will be transitioning to other support in the next year.
- Cross-Directorate Collaborations—The Postdoctoral Program also collaborates with other directorates to find strategic personnel that can address areas of mutual interest. Also, utilization and interaction with the Lab-wide Lawrence Fellowship Program has located several high-quality postdoctoral appointees for CMS.
- Enhance Contacts External to LLNL— The continued goal is to improve current and future contacts (e.g., academia and other national laboratories). LLNL enhances its credentials and reputation as a world-class laboratory of science when a postdoc's tenure is a positive experience. A CMS postdoc hired in an academic or industrial atmosphere becomes a future source of talent and an unofficial representative of the Directorate.

Mentoring Focus (con'td)



Undergraduate Summer Institute Program—Charles Westbrook, Director

Annually, the Laboratory co-sponsors 30 outstanding science and engineering students entering their senior year at colleges and universities throughout the nation. The students work a full summer as summer employees under the guidance of Laboratory supervisors, and then conclude with a 2-week workshop. In this workshop, the students attend lectures from prominent Laboratory program leaders and researchers, tour interesting facilities at LLNL, and complete their summer research projects (see Figure 29).

The Undergraduate Summer Institutes in Contemporary Topics in Applied Science was founded in 1985 to provide participants a unique opportunity to develop an understanding of the basic principles and the state-of-the-art in applied science. The experience provides a rare, closeup look at how "big science" is performed.

The curriculum consists of lectures and projects in such areas as laser and magnetic fusion, astrophysics, free-electron and x-ray

lasers, computational modeling, surface and interface science, solid-state chemistry and physics, biomedical sciences, metallurgy, materials science, precision engineering, neural networks, and selected topics on national security. CMS currently organizes and leads this program through CChED, providing staff research personnel a unique opportunity to work with these future scientists. The students, who are excellent students at leading American universities, are encouraged to consider returning to LLNL to carry out their graduate study research through the LLNL Student-Employee Graduate Research Fellowship Program. In addition, this program offers an opportunity to interact with faculty at the universities where these students are undergraduates, strengthening the links between LLNL/CMS and its academic colleagues.

Many past participants of the Undergraduate Summer Institute and Student Employee Graduate Research Fellowship programs have subsequently become Laboratory employees.

For additional information, see our web sites:

- Undergraduate Summer Institute Program: http://www.llnl.gov/usi
- Student Employee Graduate Research Fellowship: http://www.llnl.gov/urp/ Sefellowship/

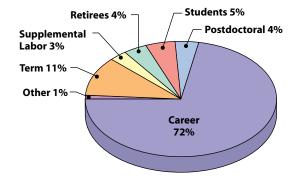


Figure 29. Students at the 2000 Undergraduate Summer Institute having lunch with LLNL Director Emeritus Edward Teller.

CMS Core Strategies

The CMS Core Strategies focus around five key subject areas:

- Science and Technology Focus—to create an integrated and balanced research portfolio and increase collaborations and visibility with potential sponsors.
- Program Focus—to create organizational design/plans to focus on program interactions.
- Workforce and Leadership Focus—CMS
 will be recognized by the Programs as vital
 to reaching their mission objectives. We
 will be organizationally agile, with a broad
 set of high caliber leaders, at all levels
 within the organization ready to step up to
 the various challenges posed by our clients.
 We will be recognized as an employer of
 choice.
- Scientific Capabilities and Infrastructure Focus—to identify and enhance key capabilities for staffing; facilities, equipment and instrumentation; and enable the processes in business, ES&H, security, and Integrated Safety Management.
- Institutional and External Focus—to increase CMS' participation in institutional planning, management and infrastructure; and expand CMS' role and influence in external scientific communities.



Staffing and Demographics

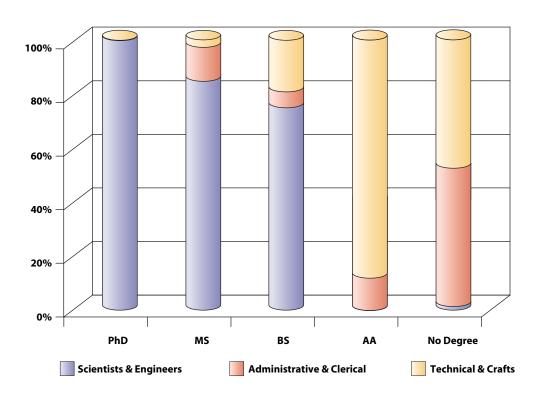
As of September 30, 2001, the CMS workforce (by head count) was 477. This workforce is comprised of 72% career, 11% term appointment, 4% postdoctoral, 4% retiree, 5% student, 1% temporary, and 3% supplemental labor (see Table 9). Table 10 shows staff profile and degree composition for career employees (by head count) is 395. The staffing breakdown is 72% scientists and engineers, 17% technicians, and 11% administrative and clerical.

Table 9. CMS Workforce.

Workforce Category	Heads	Staff%
Career	341	71%
Indefinite Full-Time Indefinite Part-Time	324 17	68% 4%
Term Appointment	51	11%
Flexible Term Full-Time Flexible Term Part-Time	49 2	10% 0%
Postdoctoral/Grad Students	20	4%
Non-Career	50	10%
Temp Student/Faculty Retiree Misc.	4 23 21 2	1% 5% 4% 0%
Total Career and Non-Career	462	97%
Other Labor Non-LLNL	15	3%
Supplemental Labor	15	3%
Total Laboratory Heads	477	100%
Minor variances may occur due Dated: September 30, 2001	to round	ing

 Table 10.
 CMS Staff Profile by Job Title and Degree Composition.

Job Title	PhD	MS	BS	AA	No Degree	Total	Staff%
Scientists & Engineers	198	33	52	_	1	284	72%
Physicist—(270)	53	2	_	_	_	55	14%
Chemist—(242)	91	16	34	_	1	142	36%
Engineer/Patent Eng.—(168, 249)	24	9	11	_	_	44	11%
Mathematician/Computer Scientist—(256, 285)	_	1	_	_	_	1	0%
Biological Scientist—(225, 277, 235, 228, 221)	_	_	4	_	_	4	1%
Environmental Scientist—(230)	_	1		_	_	1	0%
Metallurgist—(265)	30	4	3	_	_	37	9%
Administrative & Clerical	_	5	4	3	32	44	11%
Management—(196, 197)	3	_	_	_	3	1%	
Administrative—(100-162)	_	2	2	_	12	16	4%
Clerical/General Services—(400-462)	_	_	2	3	20	25	6%
Technical & Crafts	_	1	13	23	30	67	17%
Technical—(302-339, 393, 347-391, 502-588, 593)	_	1	13	23	30	67	17%
Total Laboratory Heads	198	39	69	26	63	395	100%
Degree Composition %	50%	10%	17%	7%	16%	100%	
Career Employees Only Minor variances may occur due to rounding Dated: September 30, 2001							



The breakdown within the scientific and engineering disciplines is 14% physicists, 36% chemists, 11% engineers, 9% metallurgists, and 1% biological scientists (see Table 10). About 66% of the scientists and engineers in CMS have a PhD.

The scientific staff by Discipline is shown along with postdoctoral labor in Table 11.

A discipline staff profile spanning ten years is shown in Table 12.

Table 11. CMS Scientists and Engineers by Discipline and Postdoctorals.

Job Title	Total	Staff%
Scientists & Engineers	284	93%
Physicist—(270)	55	18%
Chemist—(242)	142	48%
Engineer/Patent Eng.—(168, 249)	44	14%
Mathematician/Computer Scientist—(256, 285)	1	0%
Biological Scientist—(225, 277, 235, 228, 221)	4	1%
Environmental Scientist—(230)	1	0%
Metallurgist—(265)	37	12%
Postdoctorals	20	7%
Total Laboratory Heads	304	100%
Includes career, terms, and postdoctoral appointment. Minor variances may occur due to rounding Dated: September 30, 2001	s only	

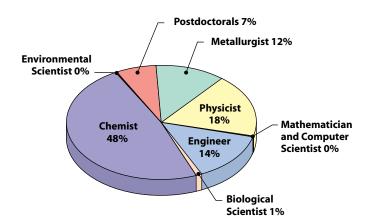
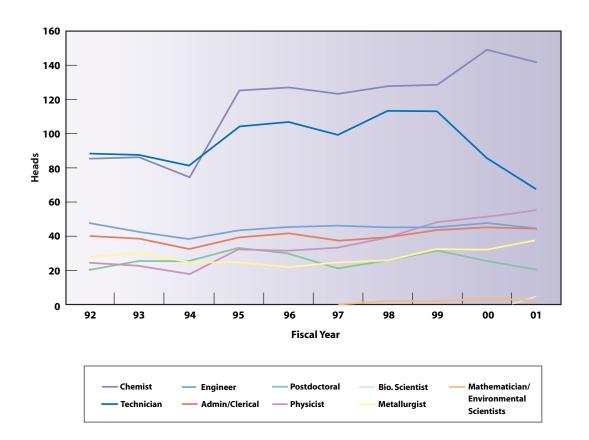


Table 12. Ten-Year CMS Staff Profile by Classification.

Discipline	1992	1993	1994	1995	1996	1997	1998	1999	2000	2001	
Chemist	85	86	74	125	127	123	128	129	149	142	
Physicist	24	22	17	32	31	33	39	48	51	55	
Metallurgist	28	30	24	25	22	24	26	32	32	37	
Engineer	47	42	38	43	45	46	45	45	47	44	
Mathematician	0	0	0	0	0	0	1	1	2	1	
Environmental Scientist	0	0	0	0	0	0	1	1	1	1	
Biological Scientist	0	0	0	0	0	0	0	0	0	4	
Postdoctoral	20	25	25	33	29	21	25	31	25	20	
Technician	88	87	81	104	107	99	113	113	85	67	
Admin/Clerical	40	38	32	39	41	37	39	43	45	44	
Total CMS (Heads)	332	330	291	401	402	383	417	443	437	415	
Excludes summer hires and supplemental labor Dated: September 30, 2001											



Financial and FTE Highlights

Figure 30 illustrates how CMS will be funded in FY02, summarized as follows:

Internal CMS Funding

- Institutional Investment—funding comes from the Laboratory General and Administrative (G&A), IGPE, LDRD collections.
- CMS Infrastructure—funding comes from CMS Directorate Program Development Charge (PMC), Organizational Facility Charge (OFC), Organizational Personnel Charge (OPC) collections and Line Item Construction.
- Discipline S&T—funding comes from DOE, federal and non-federal sponsors.
- Program Support—funding comes from CMS Scientific Service Centers collections.

Non-CMS Funding

Program Support—The Directorate primarily provides discipline personnel for support to all the Programs of the Laboratory. Support for matrixed staff to Program elements is received from other cost centers as FTE allocations.

Distribution of FTEs and Funding

Table 13 shows a distribution of CMS FTEs for FY01 and planned FY02. CMS scientific services FTEs are shown matrixed out to illustrate support to programs.

Table 14 shows how CMS managed activities are supported according to funding sources. There are four categories:

- Category 1: Discipline Science and Technology (S&T)—consists of research projects over which the Directorate has jurisdiction. In FY01, this involved 13 FTEs of CMS personnel and 7 FTEs matrixed in from other organizations for a total budget of \$8.4M.
- Category 2: CMS Infrastructure—
 consists of indirect activities involved in
 operating the Directorate. In FY01, this
 included 52 FTEs of CMS personnel and
 35 FTEs matrixed in from other organizations for a total budget of \$20.2M.
- Category 3: Institutional Investment—
 consists of indirect activities. In FY01,
 this included 29 FTEs of CMS personnel
 and 18 FTEs matrixed in from other
 organizations for a total budget of
 \$15.6M.

Figure 30. How CMS is Funded FY02 (\$K).

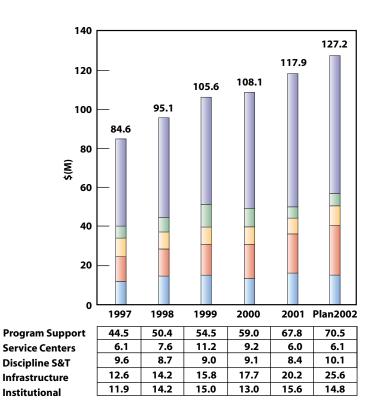
CMS Funding Source	:es
Total	127,193
Programs Support	76,643
Discipline S&T	10,110
Infrastructure	25,655
Institutional	14,785
Note: CMS managed operating and capital \$56.7	

Program Support	
Programs	76,643
282 CMS FTEs matrixed	
(other AD cost centers) Scientific Service Centers	70,500
Scientific Service Centers	6,143

Discipline S&T	
Discipline S&T	10,110
BES	3,020
BES-CE	590
Other Direct	500
WFO	6,000

CMS Infrastructure	
Infrastructure	25,655
Facilities (OFC)	7,382
Info Systems (OFC)	1,768
Personnel (OPC)	9,000
Program (PMC)	950
Line Item	6,555

Institutional Investment	
Institutional 1	4,785
G&A	8,101
Postdocs/Summer	750
LDRD-ERD	3,934
IGPE-Capital Equipment	2,000
Note: Deputy Director S&T manages LDRD Lab-wide	



• Category 4: Program Support—consists of scientific services (e.g., analytical and processing activities) supporting programs at LLNL. In FY01, this included 22 FTEs of CMS personnel and 7 FTEs matrixed in from other organizations for a total budget of \$6.0M.

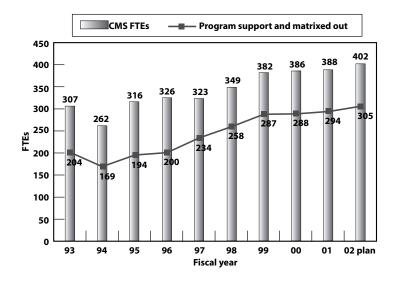


Table 13. Distribution of CMS FTEs.

	FY01	FY02 Plan
CMS Internal Programs	95	97
Discipline S&T	13	16
Infrastructure	52	52
Institutional Investment	29	29
Program Support & Matrixed Out	294	305
CMS Scientific Services	22	23
DNT	113	124
NIF-ICF	48	47
Energy & Environmental	31	31
NAI	39	40
Physics & Advanced Technology	6	5
Engineering	0	3
SS & EP	12	13
Various	23	19
Total CMS FTEs	388	402
Minor variances may occur due to rour	nding	

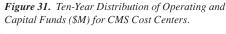
 Table 14. Distribution of Operating and Capital Funds (\$M) and FTEs for CMS Cost Centers.

	FY01 Actual 9/30/01			Planned	11/24/01	
	\$(M)	CMS FTEs	Other FTEs	\$(M)		Other FTEs
Category 1: Discipline Science & Technology	8.4	13	7	10.1	16	7
DOE-Direct	3.3	3	2	4.1	4	4
Basic Energy Sciences (KC02)	2.9	3	2	3.5	4	3
OBES Capital Equipment/Fab	0.4	0	0	0.4	0	0
Other DOE-Direct	0.1	0	0	0.2	1	1
Work for Others	5.0	10	5	6.0	12	3
WFDOE	2.0	5	1	2.0	5	1
Federal Agencies	2.7	3	4	3.6	6	2
Non-Federal	0.4	1	0	0.4	1	0
Category 2: CMS Infrastructure	20.2	52	35	25.7	52	41
Organizational Personnel Charge (OPC)	8.1	40	3	9.0	40	4
Program Management Charge (PMC)	0.9	4	0	1.0	4	1
Organizational Facility Charge (OFC)	9.2	8	32	9.2	8	36
Line Item	2.0	0	0	6.6	0	0
Category 3: Institutional Investment	15.6	29	18	14.8	29	15
General & Administrative (G&A) G&A-Special Employee Program	7.6	16	12	8.1	17	13
(Postdoctoral/Summers)	0.6	0	0	0.8	0	0
Institutional General Purpose Equipment (IGPE)	2.1	0	0	2.0	0	0
LDRD-Exploratory Research in the Disciplines (ERD)	5.3	13	6	3.9	12	2
Category 4: Program Support	6.0	22	7	6.1	23	7
Scientific Service Centers	6.0	22	7	6.1	23	7
Total CMS Operating & Capital	50.2	117	67	56.7	120	70
Minor variances may occur due to rounding						

In FY01, the sum for the CMS managed operating cost centers was \$45.7M with 184 FTEs (117 CMS and 67 matrixed in). When added to the estimated cost of personnel matrixed (272 FTEs) to support programs, the Directorate's total operating cost was about \$113.7M with a capital equipment budget of \$4.5M for a total of \$118.2M.

In FY02, the CMS managed operating cost center is expected to be \$47.9M with 190 FTEs (120 CMS and 70 matrixed in). When added to the estimated cost of personnel matrixed (282 FTEs) to support programs, the Directorate's total operating cost would be about \$118.4M with a capital equipment budget of \$8.8M for a total of \$127.2M.

Figures 31 and 32 show operating and capital costs along with FTEs from FY93 to FY02 (planned).



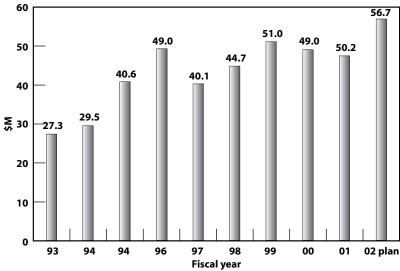
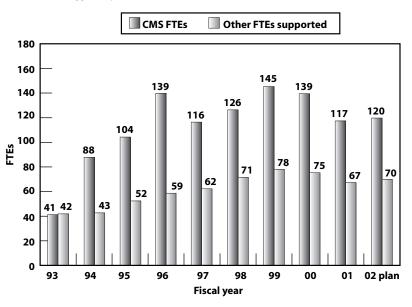


Figure 32. Ten-Year Distribution of CMS and Other FTEs Supported for CMS Cost Centers.



CMS Facilities at Site 200

Site 200 is located within the Livermore city limits on one square mile of land. CMS facilities are in the heart of the Laboratory and all facilities are within walking distance (about five minutes).

CMS has several unique chemistry facilities needed to accomplish LLNL programmatic missions. These capabilities include isotope sciences and radiochemistry diagnostics; analytical and characterization services and technology; and material and chemical process theory, modeling, and computations.

Facilities Profile

The Directorate operates four facility complexes at the Main Site: B132N, B151, B235, and B241 (see Table 15).

Table 15. Site 200 Facilities Profile.

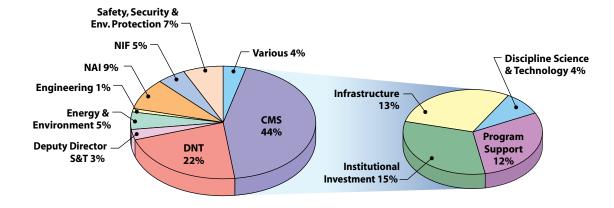
Building	Building Characteristics	Primary Functions	Major Projects	Facility Acquisition Cost
B132N/133: Chemistry Laboratories	6 years old210K gross sq. ft.Limited AccessWet Chemistry32 Labs80 Offices	 Synthesis, Formulation, and Processing Chemistry Chemical Analysis Forensics Science 		• Facility \$34M • Equipment \$12M
B151/154: Analytical & Isotopic Laboratories	• B151 34 years old B154 10 years old • 111K gross sq.ft. • Limited/Controlled Access • Wet Chemistry • 71 Labs • 123 Offices	Isotope Sciences and Radiochemistry Diagnostics Analytical and Characterization Services and Technology Geochemistry Stockpile Stewardship GTS-ITS	 Installed temporary above ground bypass of retention system drain line Began construction of B155 office building Installed T1541 office modular Completed construction of B154 HVAC upgrades Continued occupancy and activation of BSSL laboratories in B154/offices T1541 	• Facility \$49M • Equipment \$15M
B235: Materials Science Laboratories	 14 years old 91K gross sq. ft. Limited/Controlled Access Instrument Labs 30 Labs 116 Offices 	 Materials Development and Technology Material and Chemical Process Theory, Modeling, and Computation Materials Characterization Services and Technology 		• Facility \$29M • Equipment \$29M
B241: Materials Technologies Facility	 41 years old 63K gross sq. ft. Controlled Access Instrument Labs 30 Labs 1 Hi-bay 40 Offices 	 Materials Development and Technology Materials Disposition Materials Containment 	 Replaced chillers Wall-to-wall legacy equipment assessment Replaced roof 	• Facility \$21M • Equipment \$7M

OFC Collections

In FY01, OFC Collections include \$7,065K for CMS owned space (space types include: laboratory, office, cubicle, shop, inside storage, and transportainer/outside storage) and \$2,150K for Information Systems (e.g., network and central services) see Table 16.

Table 16. CMS Site 200 Space—Who Pays.

Directorate	FY01 (\$K)	%			
CMS					
Institutional Investment	1,410	15%			
Infrastructure	1,203	13%			
Discipline S&T	384	4%			
Program Support	1,141	12%			
DNT	1,981	21%			
Deputy Director S&T	236	3%			
Energy & Environment	472	5%			
Engineering	126	1%			
NAI	815	9%			
NIF	490	5%			
Safety, Security & Env. Protection	608	7%			
Various	349	4%			
Total CMS Space	9,215	100%			
Minor variances may occur due to rounding Dated: September 30, 2001					



CMS Facilities at Site 300

Site 300 is set on 7,000 acres of land about 15 miles east of Livermore. It is marked by both rolling hills and steep ravines with very few trees in sight. When it was established in 1955, Site 300 was in a very remote area surrounded only by cattle ranches. It is still remote, but today the growing city of Tracy is expanding toward the site from the east.

At Site 300, CMS facilities are divided into three groups as shown in Table 17: (1) Chemistry Area, (2) Process Area, and (3) Explosives Waste Storage Facility (EWSF) and Explosives Waste Treatment Facility (EWTF).

Chemistry Area

The Chemistry Area is used to formulate and synthesize explosives compounds, scaleup laboratory and/or bench scale size explosives formulations to production scale, and to perform precision loading of shaped charges using extrusion technology.

Process Area

The Process Area is used to produce precision explosives parts and assemblies. The area facilities contain the machine tools, isostatic presses, radiography equipment and precision assembly bays necessary for the manufacture of explosives parts.

Explosives Waste Storage Facility and Explosives Waste Treatment Facility

Explosives wastes are generated as a result of operations at Site 300 and the High Explosives Application Facility (HEAF). The explosives waste facilities at Site 300 are the EWSF and EWTF. Both of these facilities have California Department of Toxic Substances Control (DTSC) permits for the storage and treatment of explosives waste. EWSF is located in the Process Area and is used to store explosives waste for up to one year. EWTF is located at Building 845 in a remote area and is used for the open burning or open detonation of the explosives waste.

Table 17. CMS Site 300 Facilities Profile.

Facility	Facility Characteristics	Primary Functions	Capability
Chemistry Area ¹	 Average 20 years old 8 Formulations/Synthesis/ Injection/Molding 2 Mechanical Pressing Bays 3 Storage Magazines 	SynthesisFormulationMechanical PressingScaleup	 Custom manufacturing of explosives, some transferred to industry for commercialization (e.g., simulants, special operations, shaped charges)
Process Area	 Average 40 years old 6 Machine Bays 1 Inspection Bay 4 Assembly Bays 1 Radiography Bay 1 Isostatic Pressing Bay 1 Explosives Heating Bay 2 Surface Impoundments 	 Hot Isostatic Press Radiography Machining Inspection Assembly	Precision, custom manufacturing of explosives components and devices for R&D testing
Explosives Waste	 Average 40 years old—former storage magazines and shot test facility 5 Storage Magazines 1 Control bunker; detonation pad; burn cage; burn pan 	• Storage • Treatment	 State-permitted Storage Facility for 1 year storage State-permitted Treatment Facility with open burn/open detonation capabilities
	d Process Areas comprise 22 major uare feet, total equipment replace:		nes, 8 service magazines,

⁶³

Research Administration and Funding

Research is considered an integral part of the Directorate's discipline development. Oversight and policy-making are vested in the AD's office. Currently, the Deputy AD for Science and Technology assumes general responsibility for administering the research effort with guidance from the AD and consultation with Division Leaders and Program Leaders. Programs and projects are reviewed internally as well as externally. Funding for research and development that is managed in the Directorate comes primarily from LDRD, DOE Office of Basic Energy Services (DOE/OBES), and Reimbursable/WFO.

Laboratory Directed Research and Development (LDRD)

The DOE has issued an Order to provide for an LDRD Program that will allow the use of an annual percentage of the Laboratory's budget for discretionary research (6% for FY01). The LDRD Program at LLNL is divided into three major funding categories: Strategic Initiatives (SIs); Exploratory Research in the Disciplines (ERD), Programs, and Institutes; and Laboratory-wide (LW) Competition.

Strategic Inititatives (SI)

An SI project should describe innovative research and development activities that are likely to set new directions for existing programs, will help develop new programmatic areas within our mission responsibilities, and/or will enhance the Laboratory science and technology base. An SI project must have the active support of at least one of the four Laboratory Strategic Councils. In the realm of SIs, the Directorate usually participates as a key member of a team on a Program-sponsored initiative rather than directly leading one, although exceptions to this do occur.

Exploratory Research in the Disciplines (ERD), Programs and Institutes

These research and development activities are intended to support pioneering research and development projects that set new directions for the Laboratory and/or enhance the core competencies and the science and technology base for the Laboratory. The Exploratory Research in the Programs is funded by R&D collections returned to the directorates that generate the funds. Such funds are designated to provide the technical base for developing both existing and future programs for the Laboratory. CMS frequently plays a role in these projects, through personnel supporting the execution of the science and occasionally by providing the leader for the project. In general, support for a project is limited to, at most, three consecutive years in this Program. Table 18 shows FY02 CMS ERD projects.

The primary focus of CMS within its LDRD ERD portfolio is to support the longer-range research objectives of the Laboratory's Programs. CMS influences the direction and development of these objectives by contributing to new science and capabilities. Two strategic objectives define how CMS uses its ERD portfolio:

- 1. Program-related ERD. Fundamental research that provides a basic scientific understanding of a specific issue faced by a program and acknowledged by the program as being important. CMS refers to this as program-related LDRD and, in many cases, CMS is successful in getting the programs to co-invest their LDRD funds on these projects. Table 18 summarizes program-related CMS projects and associated programmatic co-investments.
- 2. New Scientific Capabilities. Development of new science and capabilities focused on chemistry that will seed enduring, externally funded, fundamental science in areas of current or future importance to the Laboratory. CMS refers to this grouping of projects as new scientific capabilities. In some cases, these projects represent a new focus area such as Biochemistry and Health Sciences shown in Table 18.

 $\textbf{\textit{Table 18.} CMS FY02 LDRD Projects and Funding Levels.}$

CMS Contact	Project [*]	Title	Funding \$K	Directorate Co-Funded
	Explora	tory Research in the Disciplines (ERD)		
	Progran	n Related ERD—DNT		
Allen	_	Thermodynamics and Structure	\$156	\$360
Campbell		Shear Localization and Fracture i	\$140	\$345
Balazs	01-ERD	Life-Performance	\$108	\$133
Schwartz	01-ERD	Metastability and Delta-Phase Retention	\$160	\$335
	Progran	n Related ERD—NAI		
Reynolds	01-ERD	Nanoscience and Nanotechnology	\$75	\$200
Westbrook		Local-Scale Atmospheric Reactive-Flow Simulations	\$130	\$150
Gard	02-ERD	Single Cell Proteomics with Ultra-High-Sensitivity Mass Spectrometry	\$200	\$270
	Progran	n Related ERD—Energy & Environmental		
Wirth	01-ERD	A Combined Multiscale Modeling and Positron Characterization Approach	\$125	\$100
Kertsting	00-ERD	Colloidal Transport of Actinides	\$125	
-		entific Capabilities—Computational Chemistry		
Melius	02-ERD	Multiscale Modeling of the Chemical Reactions	\$200	\$56
A. Quong		A 3-D Model of Signaling and Transport Pathways in Epithelial Cells	\$200	
Balasubramanian	02-ERD	Computational Actinide Chemistry at Mineral Interfaces and Colloids	\$115	
	New Sci	entific Capabilities—Biochem/Health Services		
Shields	00-ERD	Structural Characterization of Noncovalent Interactions	\$200	
De Yoreo	01-ERD	Dip-Pen Nanolithography for Controlled Protein Deposition	\$360	
Hollars	02-ERD	Development of Ultra-Sensitive High-Speed Biological Assays	\$100	\$200
Perkins	01-ERD	Development of Synthetic Antibodies	\$225	
J. Quong	01-ERD	Imaging and Dose Estimation	\$225	
	New Sci	entific Capabilities—Laser Materials Interactions		
Balooch	01-ERD	Femtosecond Laser Synthesis of Multi-Element Nanocrystals	\$200	
Kalantar	01-ERD	High-Pressure, High-Strain Rate Materials Effects	\$100	\$90
	New Sci	entific Capabilities—Nanoscience		
Van Buuren	00-ERD	Smart Membranes	\$215	
Nieh	01-ERD	Enhancement of Strength and Ductility	\$225	
	New Sci	entific Capabilities—General		
Schuh	02-ERD	Grain Boundary Character	\$50	
Moody	02-ERD	Investigation of the Shores of the Island of Stability	\$250	
Bakajin	02-ERD	Fast Microfluidic Mixer for Studies of Protein Folding Kinetics	\$50	
	Total ER	D	\$3,934	\$2,239
	Laborat	ory-Wide Competition (LW)		
Taylor	00-LW	Quantum Dots-Surface Modification & Novel Electronic Properties		\$178
Huser	00-LW	Surface-Enhanced Raman Spectroscopy		\$180
Noy	01-LW	Direct Imaging of DNA-Protein Complexes		\$190
Vance	01-LW	Surface Attachment		\$172
Baumann	01-LW	Three-Dimensional Nanoscale Structures		\$147
Hollars	01-LW	Single-Molecule Techniques		\$184
Maxwell	01-LW	Solid-State NMR Methods		\$179
Glaesemann	02-LW	Quantum Vibrations in Molecules		\$116
Shields	02-LW	Photoluminescent Silica Sol-Gel		\$186
	Total LW	I		\$1,531

CMS' selection process focuses on projects meeting these strategic objectives but also considers several other important criteria:

- Projects must be based on the execution of excellent science.
- Whenever possible, projects should provide an opportunity for our more experienced scientists to work with our younger staff, and especially postdoctoral students, in a mentoring relationship.
- Partnering/collaboration with other directorates is encouraged in all areas, and required for program-related research.

Laboratory-wide (LW) Competition

Projects in this category emphasize innovative research concepts and ideas with limited management filtering to encourage the creativity of individual researchers. Table 18 also includes nine projects funded from Labwide Competition (managed by the Laboratory's S&T Deputy Director).

DOE Direct

The Directorate coordinates funds obtained from the Office of Basic Energy Sciences, Division of Materials Sciences (OBES/DMS), which totaled \$3.0M for FY02 (see Table 19). In addition to execution of the majority of the program, this includes reporting, oversight and review for the entire program. The Livermore OBES/DMS Program has three major components:

- Metallurgy and Ceramics Program—
 addresses a diverse range of topics
 including adhesion and bonding at internal
 interfaces, fundamental characterization
 and modeling of welding processes, as well
 as research focused on the fundamentals of
 superplastic deformation.
- Solid-State Physics Program—has three components addressing new concepts in modeling radiation damage in solids, the development and characterization of new optical materials including new lasing materials, and the development of positron science as a key materials characterization technique.

Table 19. CMS FY02 OBES Projects and Funding Levels.

Contact	Project Title	Operating \$K	Capital \$K
Materials Science			
Diaz de la Rubia	Radiation Damage	218	
Elmer/Wong	Welding Metallurgy Group	446	
Campbell/King	Adhesion & Bonding at Internal Interfaces Studies	282	
Terminello	Galileo Detector Capital Equipment		540
Terminello	ESCA 2000		50
Terminello	Center of Excellence Synthesis Processing	83	
Nieh	Interfaces & Interphases on Superplasticity	422	
Terminello	Microstructural Effects on Mechanics of Materials	50	
A. Quong	Physical Properties	68	
Fox	Advanced Materials for Polymers	18	
Terminello	Growth & Formation of Advanced Heterointerfaces	376	
Tobin	Investigation of Nanoscale Magnetics	395	
Total CMS OBES		\$2,358	\$590
Other			
Howell/Tobin	PAT—Positron Research	249	
Payne	LS&T—Optical Materials	413	
Total Other OBES		\$662	
Grand Total OBES		\$3,020	\$590

Materials Chemistry
 Program—addresses the
 science of thin buried layers
 and the exploration of innova tive new techniques for
 characterizing magnetic
 properties at the atomic level.

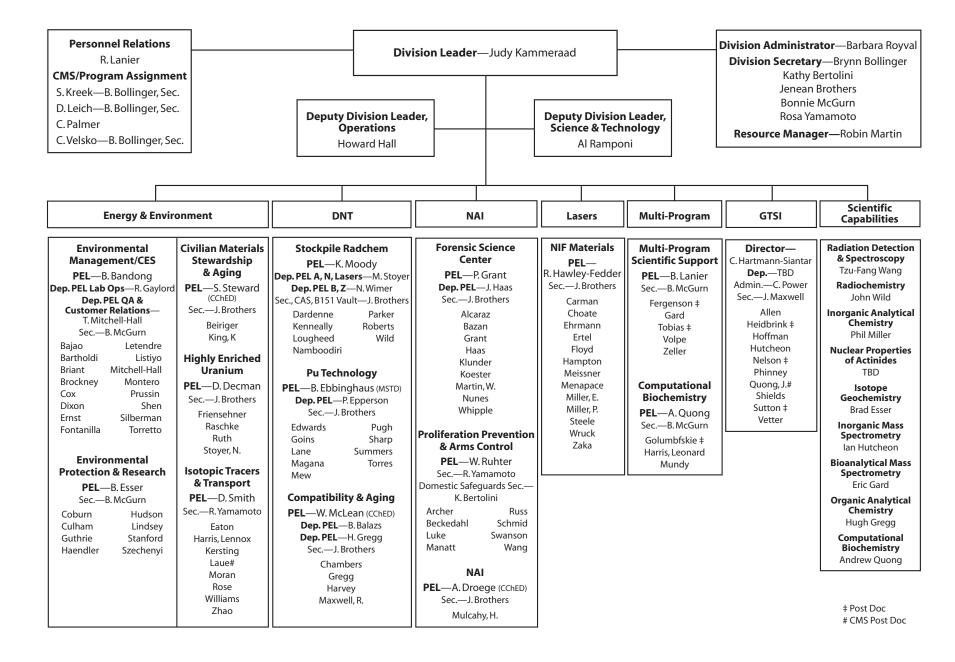
Scientific and Technical Achievements

Table 20 lists the Directorate scientific and technical achievements for the 2001 calendar year.

Table 20. Scientific and Technical Achievements (Jan-Dec 01).

Metric	Jan-Dec 01 Appraisals
Major Awards	7
R&D 100 Awards	1
Patent Disclosures	14
Patent Applications	15
Patents Issued	14
Licenses Executed	2
Refereed Publications	221
Invited Presentations (major	conferences) 71
Contributed Presentations	100
Journal Editorships	9
Conferences Organized	7
Editorial Boards	6
Citations	1

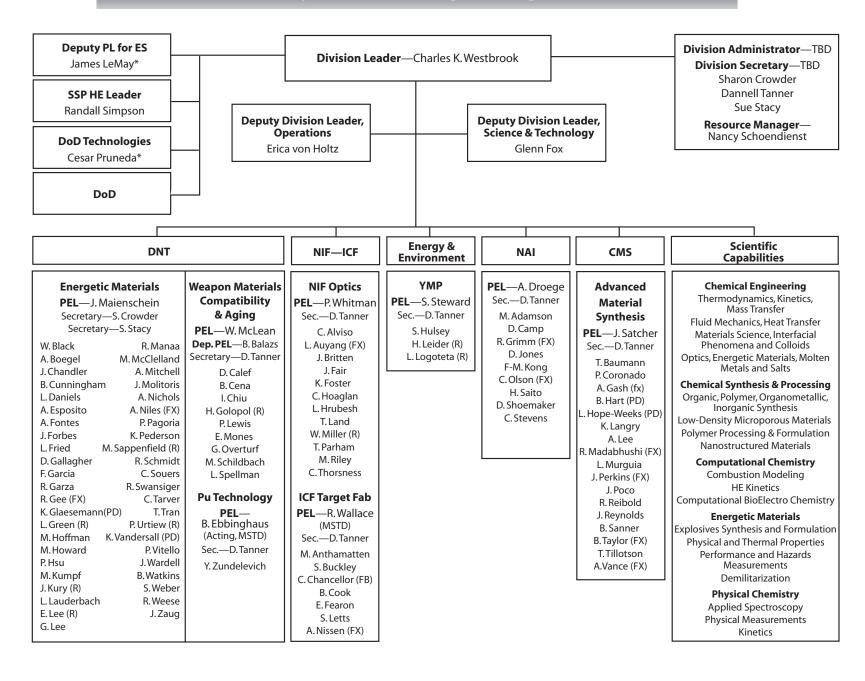
Analytical & Nuclear Chemistry Division



Analytical & Nuclear Chemistry Division Scientific Capabilities

Rad Detection & Spectroscopy	Radiochemistry	Inorganic Analytical Chemistry	Nuclear Properties of Actinides	Isotope Geochemistry	Inorganic Mass Spectrometry	Organic Analytical Chemistry	Bioanalytical Mass Spectrometry	Computational Biochemistry
Tzu-Fang Wang	John Wild	Phil Miller	TBD	Brad Esser	Ian Hutcheon	Hugh Gregg	Eric Gard	Andrew Quong
Archer Bandong Beckedahl Decman Friensehner Harris, Lennox Kammeraad Kreek Luke Manatt Parker Raschke Ruhter Ruth Vetter	Cox Dixon Fontanilla Gaylord Grant Guthrie Laue Lougheed Moody Namboodiri Palmer Prussin Roberts Shen Stanford Stoyer, N. Summers Sutton Szechenyi Torretto Williams Zhao	Bartholdi Bajao Brockney Briant Carman Edwards Epperson Ernst Floyd Goins Haendler King, K. Klunder Lane Letendre Magana Miller, E. Silberman Sharp Steele Swanson Torres Wruck	Allen Dardenne Hall Lanier Schmid Stoyer, M. Wimer	Kenneally Kersting Rose Smith Volpe	Beiriger Culham Eaton Hudson Leich Miller, P. Moran Phinney Pugh Russ Velsko Zaka	Alcaraz Chambers Choate Coburn Ehrmann Ertel Floyd Haas Hampton Harvey Hawley-Fedder Koester Lindsey Listiyo Maxwell Meissner Mew Mitchell-Hall Mulcahy Nunes Whipple	Fergenson Quong. J. Shields Tobias Zeller	Golumbfskie Harris, Leonard Mundy

Chemistry & Chemical Engineering Division

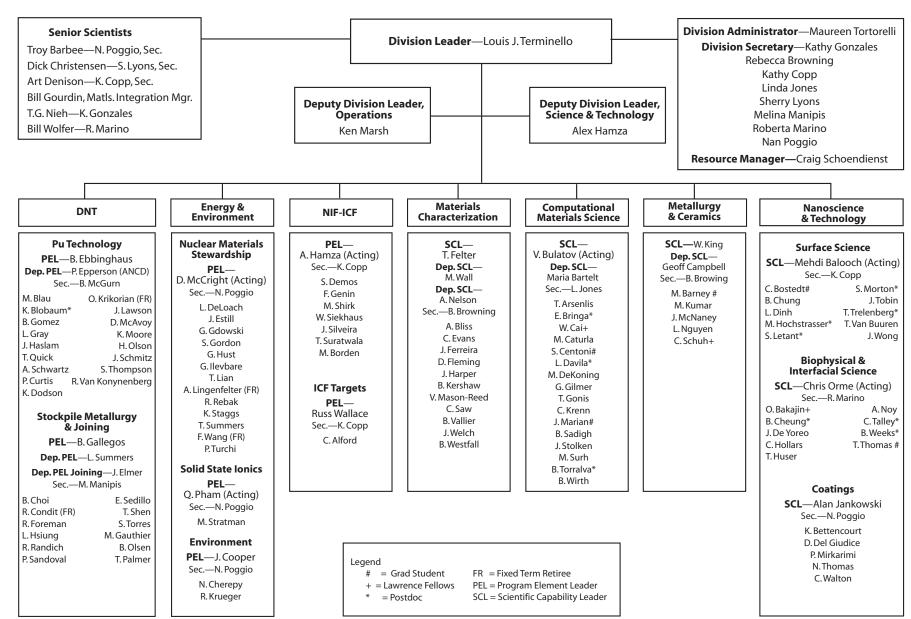


Chemistry & Chemical Engineering Division Scientific Capabilities

Chemical Synthesis & Processing	Chemica	Chemical Engineering		Chemistry	Computational Chemistry	Energetic Materials*	
SCL—J. Satcher	SCI	SCL—TBD		TBD	SCL—C. Westbrook	SCL—J. Maienschein	
S. Gam Polymers A. Gash	(PD) L. Auyang J. Britten D. Camp R. Cena B. Cunninghan D. J. Fair K. Foster C. Hoaglan L. Hrubesh ry P. Hsu P. Hsu D. Jones F-M. Kong F-M. Kong Ser It* X)	n J.Maienschein* M.McClelland* W.Miller (R) T.Parham M.Riley D.Shoemaker C.Thorsness T.Tran* B.Watkins* P.Whitman Y.Zundelevich	Applied Spectroscopy A. Droege R. Grimm T. Land C. Olson H. Saito (FX) C. Stevens J. Zaug* General Physical Chemistry M. Adamson E. Fearon J. Forbes* R. Garza* S. Hulsey H. Leider (R) L. Logoteta (R) A. Nissen (FX) S. Steward R. Swansiger*	Materials Compatibility B. Balazs I. Chiu H. Golopol (R) J. LeMay P. Lewis W. Mclean E. Mones J. Nielsen G. Overturf* M. Schildbach L. Spellman	K. Balasubramanian D. Calef L. Cloutman R. Cook L. Fried* M. Howard* A. Kubota (PD) R. Manaa* C. Melius A. Miller M. Murphy* A. Nichols* W. Pitz C. Schaldach C. Souers* J. Sturgeon C. Tarver* P. Vitello* J. Young (FX)	W. Black A. Boegel J. Chandler B. Cunningham L. Daniels A. Esposito (PD) J. Forbes L. Fried F. Garcia R. Garza R. Gee (PD) K. Glaesemann (PD) L. Green (R) M. Hoffman M. Howard M. Kumpf J. Kury (R) L. Lauderbach E. Lee (R) G. Lee R. Manaa M. McClelland A. Mitchell	J. Molitoris A. Nichols A. Nichols A. Niles G. Overturf P. Pagoria K. Pederson M. Sappenfield (R) R. Schmidt R. Simpson C. Souers R. Swansiger C. Tarver T. Tran P. Urtiew (R) K. Vandersall (PD) P. Vitello J. Wardell B. Watkins S. Weber R. Weese J. Zaug

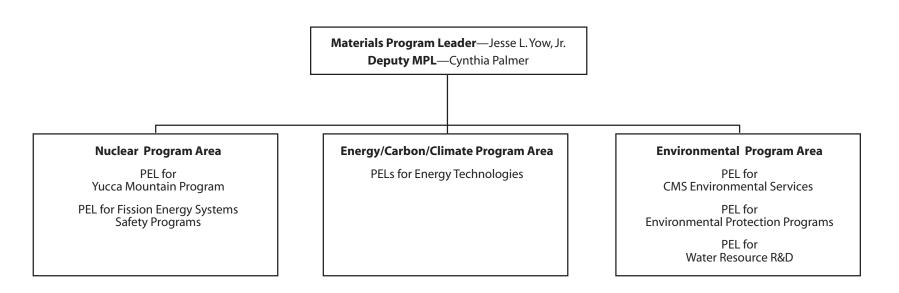
^{*} Some people in Energetic Materials have been double counted.

Materials Science & Technology Division

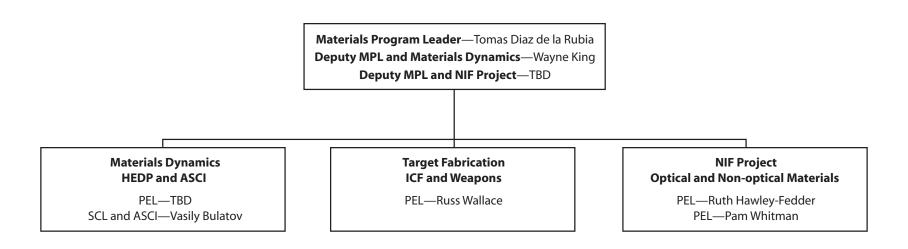


Scientific capabilities for MSTD are not available.

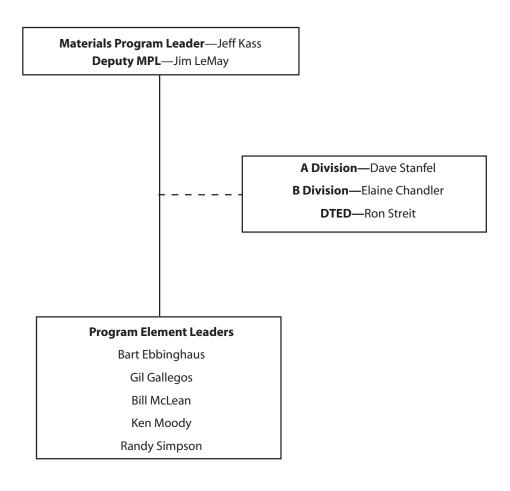
Energy & Environment Materials Program Office



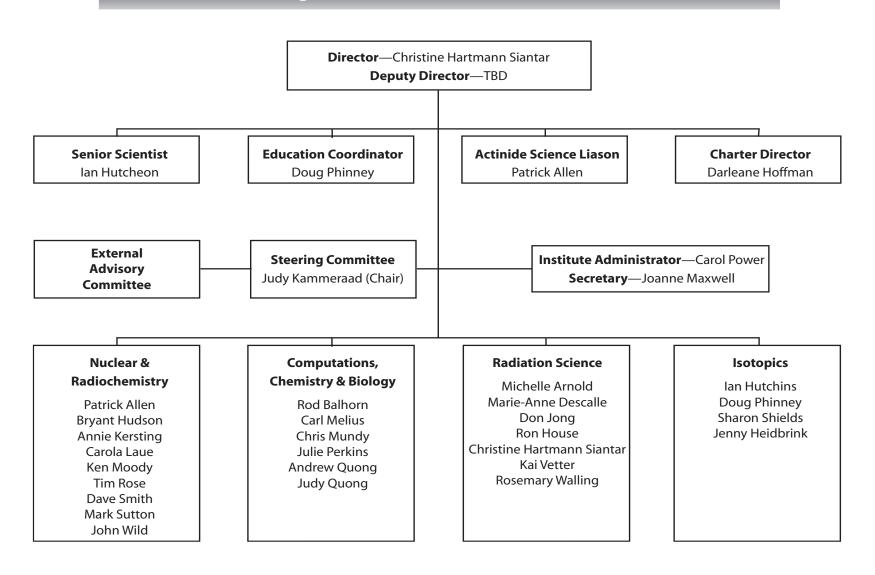
National Ignition Facility Materials Program Office



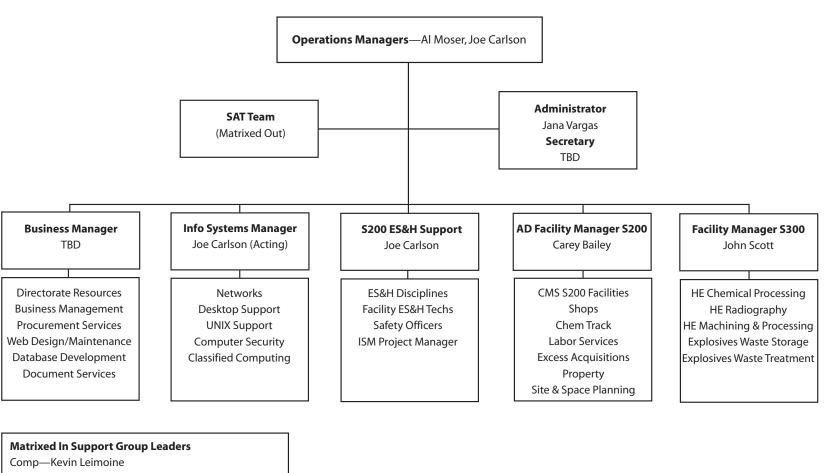
Stockpile Stewardship Materials Program Office



Glenn T. Seaborg Institute for Transactinium Science at LLNL



Operations



EE—Tony Lavietes/Mark LaChapell

ME—Moe Dehghani (Acting)/Steve Santor/Larry Walkley

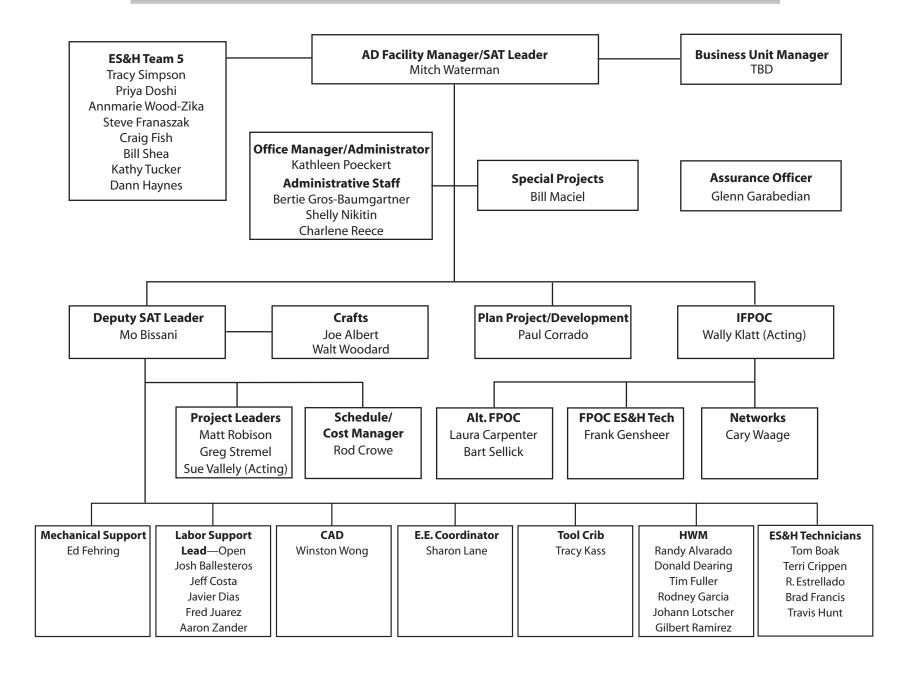
HC S200—Steve McConnel

HC S300—Ross Wilson/Jerry Bardecker

HWM—Jim Anson

Sec. Rep.—Michel Dahlstrom

Space Action Team (SAT)



Chemistry and Materials Science Current Scientific Advisory Review Committee Members

(all information from American Men and Women of Science and public web sites)

Neil Ashcroft

Professor Ashcroft has been a full Professor of Physics at Cornell University since 1974, and the Associate Director of the Cornell High Energy Synchrotron Source since 1978. He received his PhD in physics from Cambridge University in 1964. He has served on a wide variety of advisory panels and committees for DOE, NAS, academia and the APS. He is a fellow of the American Physical Society and the American Association for the Advancement of Science. His research interests are in the areas of classical and quantum liquids, optical properties of solids and theory of the metallic state.

Robert A. Beaudet

Dr. Beaudet is a Professor of Chemistry at the University of Southern California which he joined in 1962. He received his PhD from Harvard University in 1963. His awards and honors include Visiting Professor at the Max-Plank Institute for Laser Research, Alexander Von Humboldt Special Award, A. P. Sloan Foundation Research Fellow, National Bureau of Standards Research Fellow, and National Science Foundation Predoctoral Fellow. Dr. Beaudet currently chairs a NRC/NAS standing committee that has published a study entitled "Review and Evaluation of Alternative Technologies for Demilitarization of Assembled Chemical Weapons (ACW)." His research interests include infrared spectroscopy of Van der Waals clusters; remote laser detection; microwave and laser spectroscopy; molecular structure and properties of boron compounds; the structure and dynamics of weakly bonded complexes; and the structure, properties, and theory of gaseous free radicals. Dr. Beaudet is also currently a member of the NAI Directorate Review Committee.

Clyde L. Briant

Professor Briant is a full Professor of Engineering at Brown University which he joined in 1994 following 18 years as a Staff Metallurgist at the General Electric Research and Development Center. Prof. Briant received his ScD in Engineering from Columbia University in 1974. He was awarded the Robert Lansing Hardy Gold Medal and the R. W. Raymond Award by the AIME. His research interests focus on grain boundary chemistry, hydrogen embrittlement and stress corrosion, nucleation theory, and chemical bonding in alloys.

Thomas B. Brill

Professor Thomas Brill has been a full Professor of Chemistry at the University of Delaware since 1979, and on the faculty since 1970. He received his PhD in chemistry from the University of Minnesota in 1970. He was acting chairman of the department in 1985-1986 and concurrently consulted for Morton-Thiokol, CDS Instruments and Conoco Oil. Professor Brill's research interests include infrared and Raman spectroscopy, organometallic chemistry, and thermal decomposition.

Chemistry and Materials Science Scientific Advisory Review Committee Members (cont'd)

Morton M. Denn

Professor Morton M. Denn is currently a Professor of Chemical Engineering at the Levich Institute, City University of New York. He was formerly a Professor of Chemical Engineering at the University of California/Berkeley since 1981, and prior to that was the Allan P. Colburn Professor of Chemical Engineering at the University of Delaware. He received his PhD in chemical engineering from the University of Minnesota in 1964. He has been a visiting faculty member at several other institutions. He is a member of the National Academy of Engineering and a fellow of the American Institute of Chemical Engineers. His research interests include polymer processing, fluid mechanics, and process simulation.

John L. Emmett

Dr. Emmett founded JLE Associates in 1989 and continues as its president. Prior to that he was the Associate Director for Lasers at the Lawrence Livermore National Laboratory and has served on the Board of Directors of the Hoya Corporation and as president of the Crystal Research Society. Dr. Emmett received his PhD in physics from Stanford University in 1967. He received the E. O. Lawrence Award in 1978, and is a Fellow of the American Physical Society. His area of research is solid state lasers.

Kelvin Lynn

Professor Lynn has been a full Professor of Physics and Director of the Center for Materials Research at Washington State University since 1997. Prior to that was a physicist at Brookhaven National Laboratory since 1974, and head of the Materials Science Division when he departed. He received his PhD in Materials Science from the University of Utah in 1974. He has been associated with Bell Laboratories, the State University of New York at Stony Brook, and the University of Guelph, Ontario.

Elton N. Kaufmann

Dr. Kaufmann is currently the Associate Director, Strategic Planning Group at the Argonne National Laboratory, and previously led the Materials Division at Lawrence Livermore National Laboratory. He received his PhD in physics from the California Institute of technology in 1969. He is a Fellow of the American Physical Society, a past editor of Hyperfine Interactions and a former president of the Materials Research Society. His research has focused on nuclear spectroscopic methods, ion implantation and materials modification, and superconductivity.

Chemistry and Materials Science Scientific Advisory Review Committee Members (cont'd)

J. William Morris, Jr.

Professor Morris has been a full Professor of Materials Science at the University of California/Berkeley since 1977 as well as senior scientist at the Lawrence Berkeley Laboratory since 1971. He received his ScD in Materials Science from the Massachusetts Institute of Technology in 1969 and worked as a research scientist for Bell Aerospace Co. from 1968 to 1971. He was chairman of the TMS-AIME Chemistry and Physics of Metals Committee from 1978 to 1980, and is a fellow of the American Society of Metals. His research interests include alloy development, lightweight structural alloys, and high field superconductors.

William D. Nix

Professor Nix has been a full Professor of Materials Science at Stanford University since 1972, the Lee Otterson Professor of Engineering since 1989, and a member of the faculty since 1963. He received his PhD in materials science from Stanford University in 1963. Professor Nix is a member of the National Academy of Engineering, a fellow of the American Society of Metals, and a fellow of the American Institute of Mining, Metallurgical and Petroleum Engineers. He has received a variety of awards including the Mathewson Gold Medal (AIME), the Stoughton Award (ASM), and the Mehl Medal. His research interests include dislocation theory, mechanical properties of crystals and thin films, and high temperature creep and fracture.

Alfred P. Sattelberger

Dr. Sattelberger is currently the Division Director of the Chemical Sciences and Technology Division at the Los Alamos National Laboratory, and was formerly the Director of Science and Technology Base Programs and the Director of Energy Research Programs. He received his PhD in Inorganic Chemistry from Indiana University in 1975. His research interests include actinide coordination and organometallic chemistry, and homogeneous and heterogeneous catalysis.

Thomas A. Tombrello

Professor Tombrello has been a full Professor of Physics at the California Institute of Technology since 1971, specializing in surface science and planetary science. He is currently the Chairman of the Department of Physics, Mathematics and Astronomy. He received his PhD in physics from Rice University in 1961. He has been a distinguished visiting professor at the University of California/Davis, a recipient of the Alexander von Humboldt award in 1984 and is a Fellow of the American Physical Society. He served as Vice-president & Director of Research at Schlumberger-Doll Research from 1987 to 1989. He has been the Associate Editor of Nuclear Physics since 1972 and of Nuclear Science Applications since 1979. His research interests include surface physics, nuclear physics, and space physics.

Chemistry and Materials Science Scientific Advisory Review Committee Members (cont'd)

Linda K. Trocki

Dr. Trocki is Executive Vice President for Strategic Planning and Technology Commercialization for Bechtel BWXT at the Department of Energy's Idaho Engineering and Environmental Laboratory. She led Bechtel Corporation's research and development group, serving as Vice President in Bechtel National, Inc, following a 20-year career at Los Alamos National Laboratory (LANL). Dr. Trocki's research work at LANL included cost-benefit analysis, environmental restoration, and policy analysis for the Department of Energy and the US Agency for International Development. On loan during her career at LANL, she worked as Special Assistant to the Deputy Secretary of Energy in Washington, DC, on the energy R&D portfolio, and oil and gas issues. Her technical areas of expertise are in earth sciences and resources, energy and environmental systems, and economic policy. Dr. Trochi received her PhD in Mineral Economics in 1985 from Penn State. Dr. Trocki is also currently a member of the Energy and Environment Directorate Review Committee.

Karl K. Turekian

Professor Karl Turekian has been the Benjamin Silliman Professor of Geology & Geophysics at Yale University since 1985, and the Director of the Center for the Study of Global Change since 1989. He received his PhD from Columbia University in 1955. Professor Turekian is a member of the National Academy of Science, a Fellow of the Geological Society of America, a Fellow of the American Geophysical Union, and a Fellow of the American Academy of Arts & Sciences. He served for six years as the Chairman of the Department of Geology at Yale, and has served on numerous national advisory boards and committees. His research centers on geochemistry of the radionuclides and trace elements, planetary evolution, and atmospheric chemistry.

Nicholas Winograd

Professor Winograd has been a full Professor of Chemistry at the Pennsylvania State University since 1985. Prior to that he was a full Professor of Chemistry at Purdue University from 1979 to 1984, and a member of the faculty since 1970. He received his PhD in Chemistry from Case Western Reserve University in 1970, and was a Sloan Fellow from 1974 -1977 and a Guggenheim Fellow from 1977 - 1978. His research interests are in characterization of solid surfaces using spectroscopy and secondary ion mass spectrometry.

Sidney Yip

Professor Yip has been a full Professor of Nuclear Engineering at the Massachusetts Institute of Technology since 1973, and a member of the faculty since 1965. He received his PhD in nuclear engineering from the University of Michigan in 1962. He has received the von Humbolt U.S. Senior Scientist Award, and is a fellow of the American Physical Society. His research interests center on atomistic simulation of materials properties and behavior, and phase transitions.

Richard A. Yost

Professor Richard Yost has been a full Professor of Chemistry at the University of Florida since 1989. He received his PhD in Analytical Chemistry from Michigan State University in 1979 and immediately joined the University of Florida as an Assistant Professor. His research interests focus on the development of new analytical techniques and their application to environmental, forensic, and clinical chemistry.

Acronyms

AEC	Atomic Energy Commission	LLNL	Lawrence Livermore National Laboratory
AD	Associate Director	LMOT	Laser Materials and Optical Technology
AFM	Atomic Force Microscopy	LS&T	Laser Science and Technology
ANCD	Analytical and Nuclear Chemistry Division	LW	Laboratory-wide
ASCI	Accelerated Strategic Computing Initiative	MAP	Materials Analytical Programs
ASSSP	Actinide Sciences Summer School Program	MCAP	Materials Computational, Analysis, and Processing
AVLIS	Atomic Vapor Laser Isotope Separation	ME ME	Mechanical Engineering
BBRP	Biology and Biotechnology Research Program	MPL	Materials Program Leader
BSSL	BioSecurity Support Laboratory	MPO	Material's Program Office
CAPS	Counterproliferation Analysis and Planning	MRI	Materials Research Institute
CHID	System	MS	Mass Spectrometer
CMS	Chemistry and Materials Science	MSTD	Materials Science and TechnologyDivision
CChED	Chemistry and Chemical Engineering Division	NAI	Non-Proliferation, Arms Control, and International
CE	Capital equipment	11711	Security
CEES	Council for Energy and Environmental Systems	NEPA	National Environmental Policy Act
CES	Chemistry–Environmental Services	NIF	National Ignition Facility
Comp	Computations	NNSA	National Nuclear Security Administration
CRADA	Cooperative Research and Development	NTS	Nevada Test Site
CIUIDII	Agreement	OBES	Office of Basic Energy Sciences
CVD	Chemical Vapor Deposition	OFC	Organizational Facility Charge
CW/BW	Chemical Warfare/Biological Warfare	OPC	Organizational Personnel Charge
D&D	Decommissioning, Deactivation,	OSP	Operational Safety Procedure
Bub	Decontamination and Demolition	PAT	Physics and Advanced Technologies
DL	Division Leader	PDP	Planning, Development and Personnel
DMS	Division of Materials Science	PMC	Program Management Charge
DNT	Defense and Nuclear Technologies	PPAC	Proliferation Prevention & Arms Control Program
DoD	Department of Defense	PrHA	Process Hazards Analysis
DOE	Department of Energy	Pu	Plutonium
DOE/DP	Department of Energy/Defense Program	PVD	Physical Vapor Deposition
DOL/DI DP	Defense Programs	PWP	Project Work Plan
DTSC	Department of Toxic Substances Control	QA	Quality Assurance
E&E	Energy and Environment	R&D	Research and Development
EE	Electronic Engineering	RRP	Room Responsible Person
EIR	Environmental Input Report	RTI	Returned to Institution
EMC	Energetic Materials Center	S200	Site 200 (Livermore Main Site)
ERD	Exploratory Research in the Disciplines	S300	Site 300 (Livermore Explosives Testing Site)
ERWN	Environmental Restoration Waste Management	SAR	Safety Analysis Report
ESCA	Electron Spectroscopy for Chemical Analysis	SARC	Scientific Advisory Review Committee
ES&H	Environment, Safety and Health	S&Es	Scientists and Engineers
EWSF	LLNL Explosive Waste Storage Facilities	S&S	Safeguards and Security
EWTF	LLNL Explosive Waste Treatment Facilities	S&T	Science and Technology
FDA	Food and Drug Administration	S&TR	Science and Technology Review
FSP	Facility Safety Plan	SAT	Strategic Action Team
FTEs	Full Time Equivalents	SI	Strategic Initiative
FTMS	Fourier Transform Mass Spectrometer	SS&EP	Safeguards, Security and Environmental Protection
FY	Fiscal Year	SSMP	Stockpile Stewardship Management Program
G&A	General and Administrative	SSP	Stockpile Stewardship Program
GPP	General Plant Project	SST	Scientific Safety Team
GTS-ITS	Glenn T. Seaborg–Institute for Transactinium	TEM	Transmission Electron Microscope
010 110	Science	TOFMS	Time-of-Flight Mass Spectrometer
HC	Hazards Control	TQMS	Triple-Quadrupole Mass Spectrometer
HEs	High Explosives	TRACE	Transition Region and Coronal Explorer
HEAF	High Explosives Application Facility	TRR	Technical Release Representative
HWM	Hazardous Waste Management	UC	University of California
IAEA	International Atomic Energy Agency	UCB	University of California, Berkeley
ICF	Inertial Confinement Fusion	UCDRD	University of California Directed Research &
ICP	Inductively Coupled Plasma		Development
IGPE	Institutional General Purpose Equipment	UCRL	University of California Radiation Laboratory
IS	Information System Support Team	WFDOE	Work for Department of Energy
ISMS	Integrated Safety Management System	WFO	Work for Others
ITS	(Glenn T. Seaborg) Institute for Transactinium Science		
IWS	Integration Work Sheet		
KDP	potassium dihydrogen phosphate		
LDRD	Laboratory Directed Research and Development		
	Program		